

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
 Data File : BF126255.D
 Acq On : 18 Dec 2021 15:39
 Operator : JU/CG
 Sample : M5082-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2-121-1(55-62)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126255.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	11	16	rVB	932082	1181885	16.91%	2.238%
2	2.252	24	28	36	rVB	121970	154002	2.20%	0.292%
3	5.040	493	502	515	rBV	1266269	1920813	27.49%	3.637%
4	5.440	564	570	573	rBV	5561875	6563879	93.93%	12.430%
5	5.834	633	637	641	rVB	226148	202474	2.90%	0.383%
6	6.446	734	741	744	rBV	5158347	6987938	100.00%	13.233%
7	6.816	800	804	807	rBV	1635643	1364473	19.53%	2.584%
8	7.381	893	900	903	rBV	4004267	4633262	66.30%	8.774%
9	8.098	1017	1022	1025	rBV	2067869	1932236	27.65%	3.659%
10	9.181	1199	1206	1209	rBV	5818208	6552604	93.77%	12.408%
11	9.263	1216	1220	1226	rVB2	121820	113066	1.62%	0.214%
12	9.675	1286	1290	1298	rBV6	33154	74502	1.07%	0.141%
13	9.851	1313	1320	1324	rBV	2363462	2094518	29.97%	3.966%
14	10.645	1448	1455	1458	rBV	3725238	4151647	59.41%	7.862%
15	11.298	1562	1566	1569	rBV2	69100	73226	1.05%	0.139%
16	11.333	1569	1572	1576	rVV	2180693	2009488	28.76%	3.805%
17	11.404	1578	1584	1587	rBV3	125323	152732	2.19%	0.289%
18	11.869	1660	1663	1667	rBV	407869	351362	5.03%	0.665%
19	12.751	1811	1813	1820	rVB3	77476	72567	1.04%	0.137%
20	12.927	1838	1843	1847	rBV	5014716	5946007	85.09%	11.260%
21	13.845	1994	1999	2016	rBV3	560190	1434250	20.52%	2.716%
22	13.969	2016	2020	2024	rVB	1626098	1625256	23.26%	3.078%
23	14.069	2031	2037	2047	rVB	250265	304776	4.36%	0.577%
24	14.151	2047	2051	2055	rBV	77985	72216	1.03%	0.137%
25	14.451	2099	2102	2106	rBV	86979	83982	1.20%	0.159%
26	14.504	2107	2111	2117	rBV5	37782	76116	1.09%	0.144%
27	14.757	2151	2154	2158	rVB	107145	102150	1.46%	0.193%
28	14.833	2163	2167	2170	rVB	156286	151667	2.17%	0.287%
29	15.092	2207	2211	2219	rVB	125383	137737	1.97%	0.261%
30	15.416	2261	2266	2271	rBV	1044759	1321951	18.92%	2.503%
31	15.468	2271	2275	2280	rVB	122884	161138	2.31%	0.305%
32	15.898	2343	2348	2357	rVB	107931	158677	2.27%	0.300%
33	16.015	2360	2368	2378	rBV6	75125	290205	4.15%	0.550%
34	16.392	2427	2432	2443	rVB3	77569	157792	2.26%	0.299%
35	16.980	2526	2532	2539	rVB2	52590	104178	1.49%	0.197%
36	17.668	2644	2649	2658	rVB4	39885	93036	1.33%	0.176%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

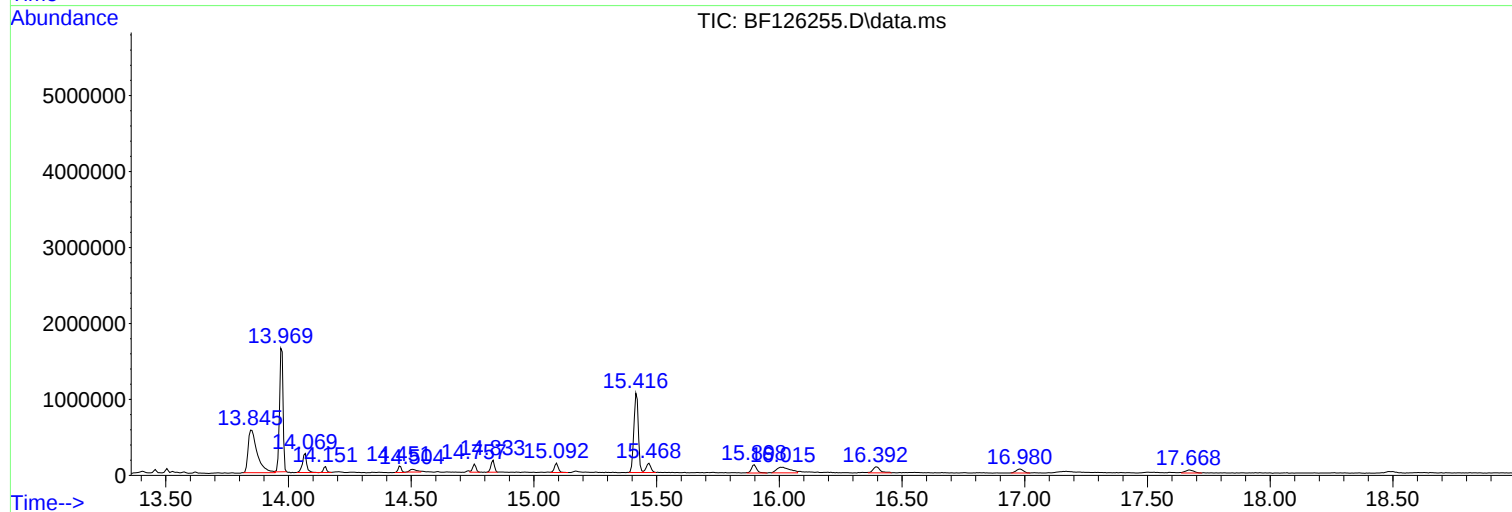
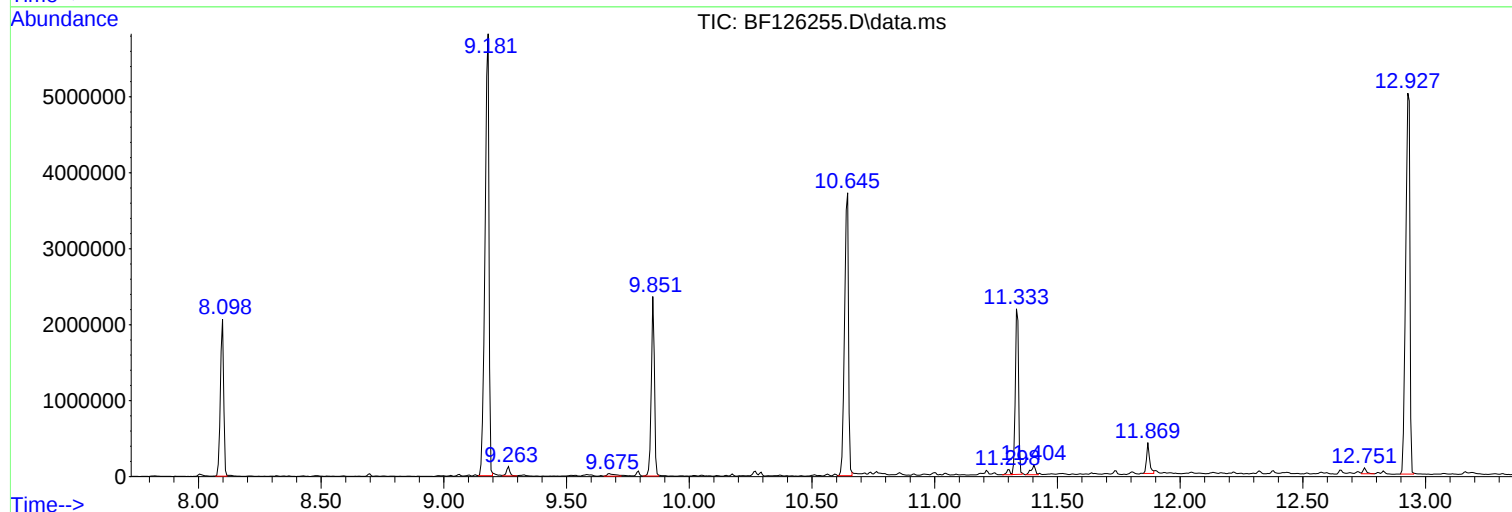
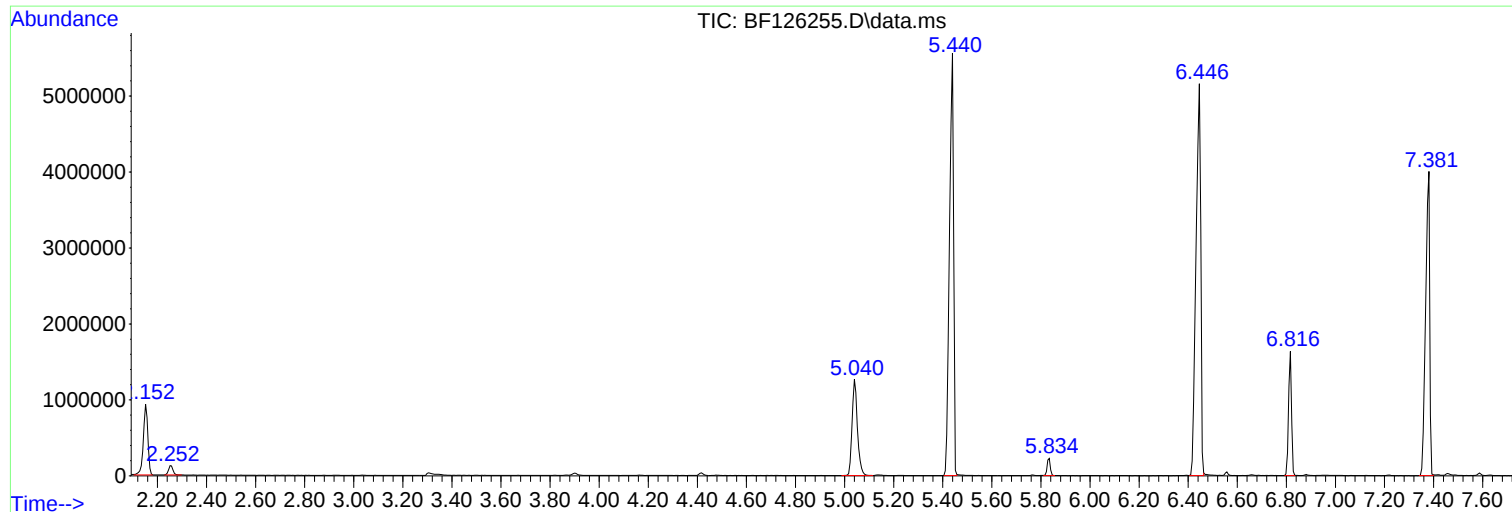
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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BNA_F
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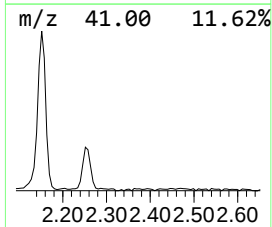
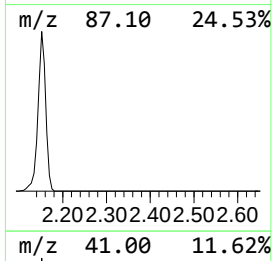
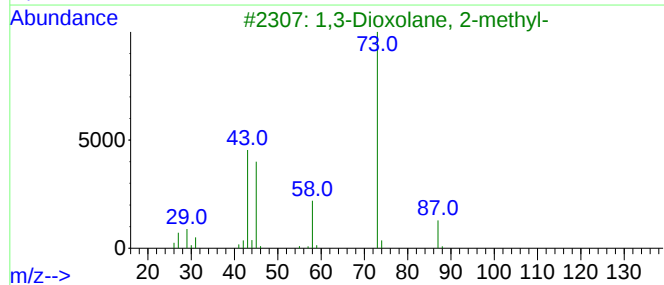
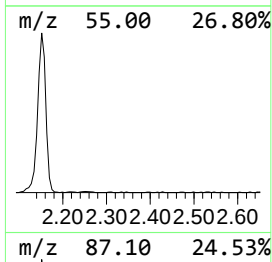
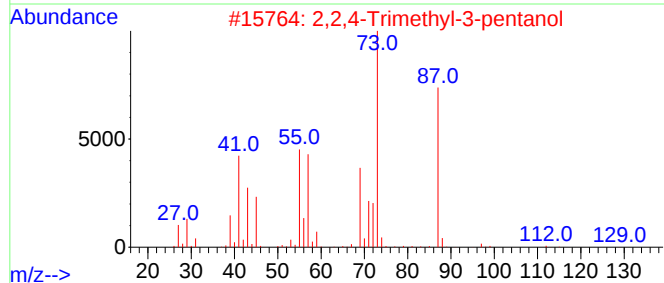
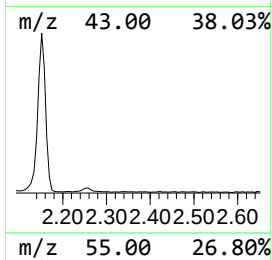
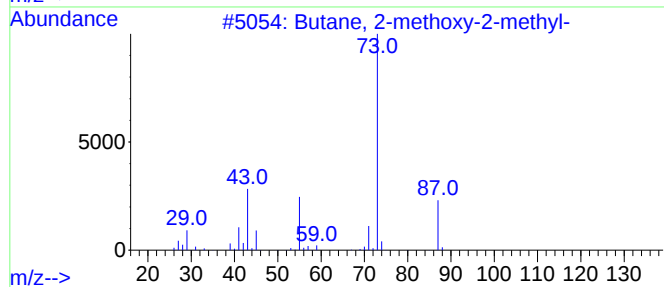
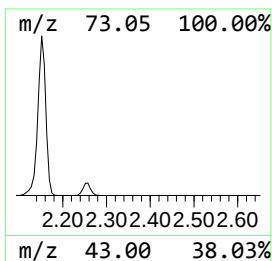
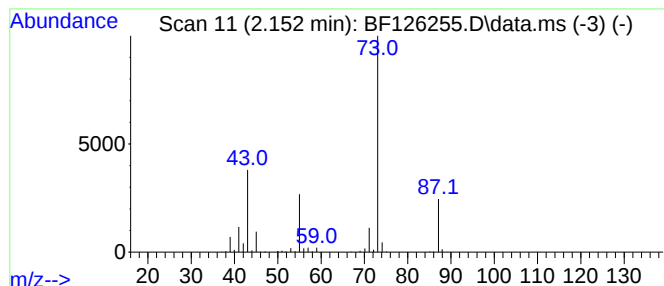
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	17.32 ng	1181890	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

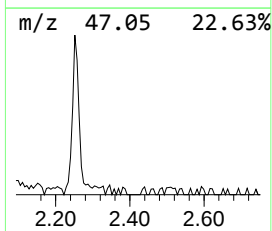
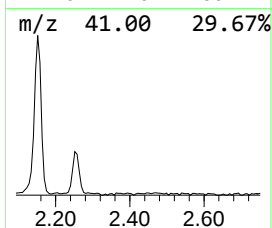
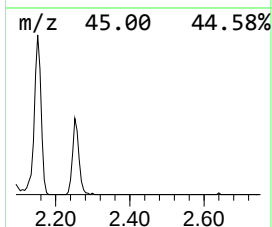
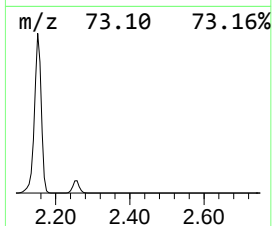
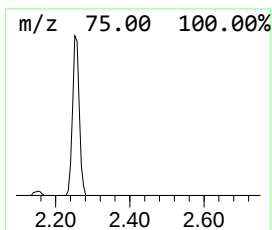
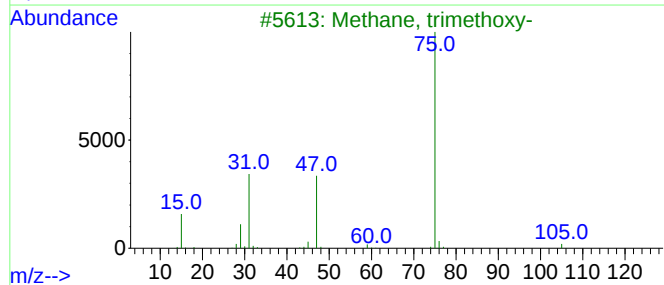
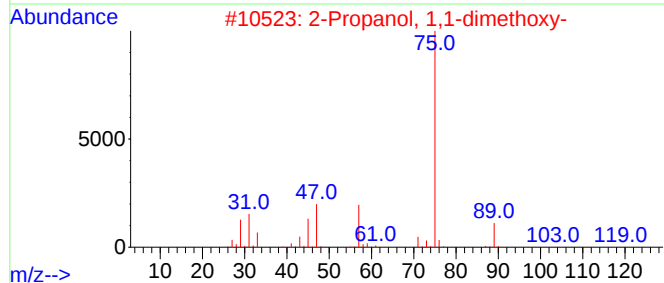
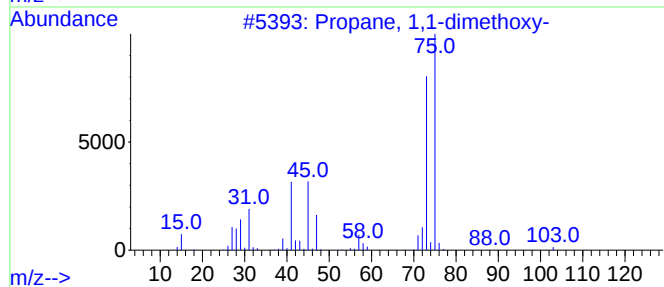
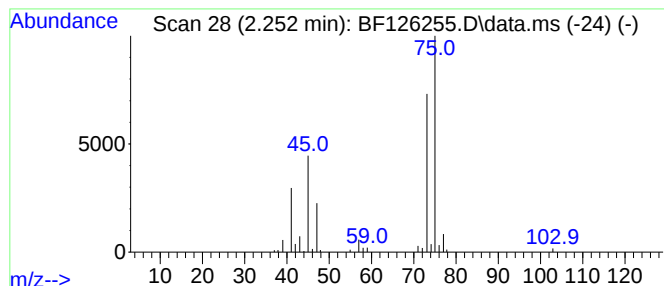
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	2.26 ng	154002	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	28
5			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28



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Misc :
ALS Vial : 9 Sample Multiplier: 1

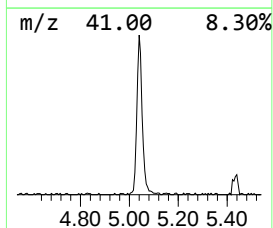
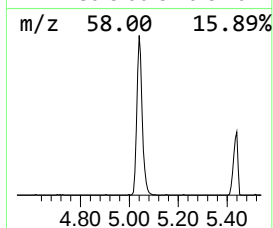
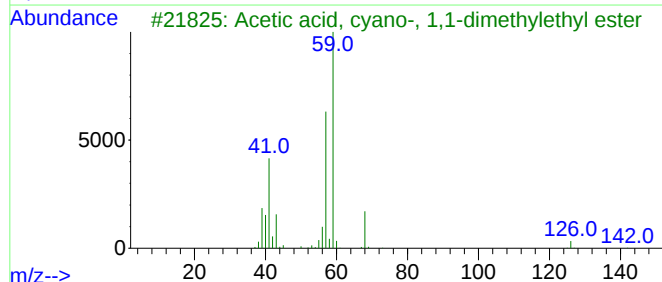
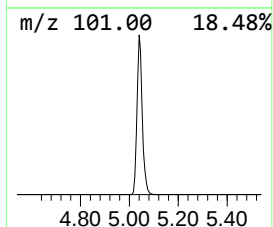
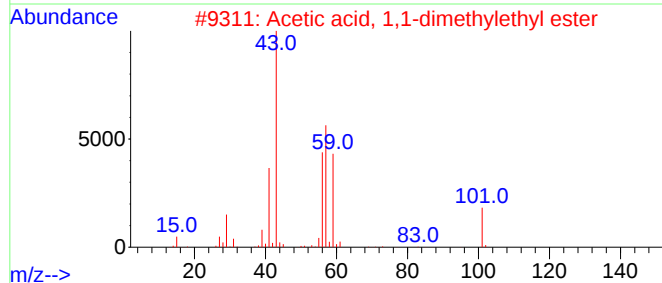
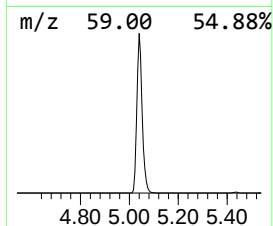
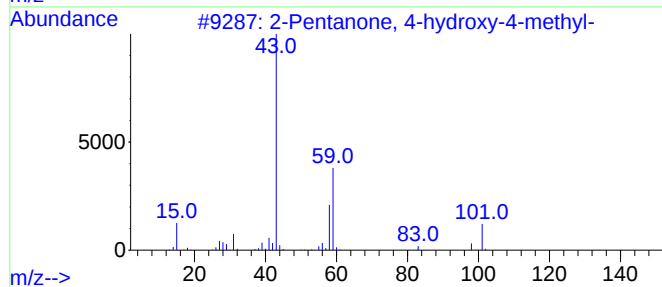
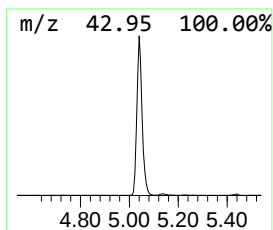
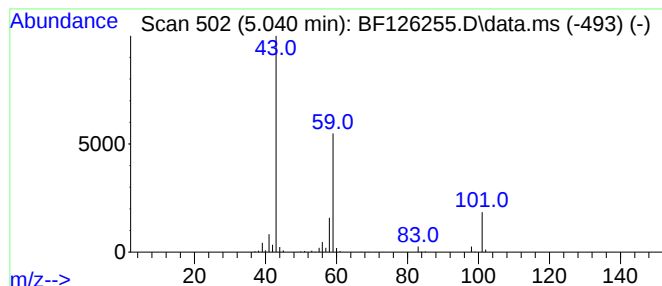
Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.040	28.15 ng	1920810	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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ClientSampleId :
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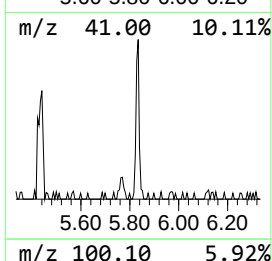
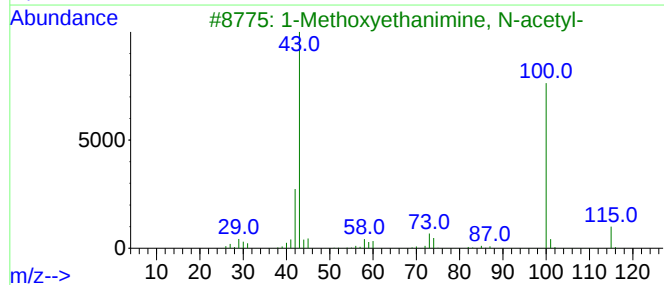
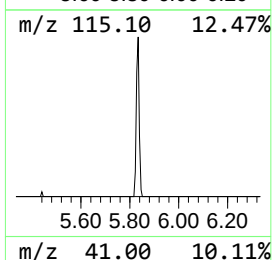
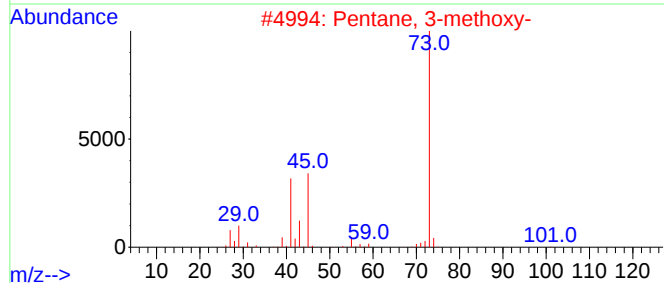
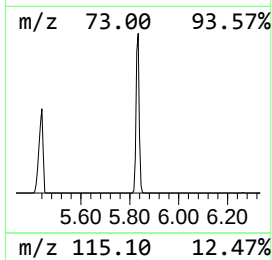
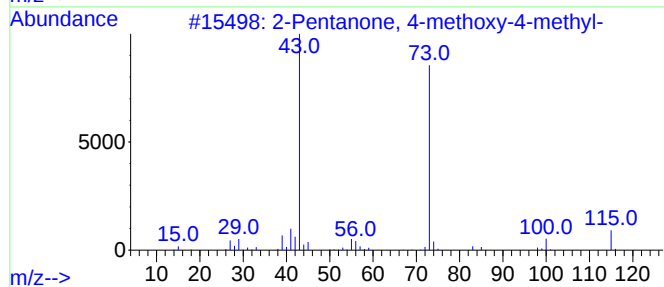
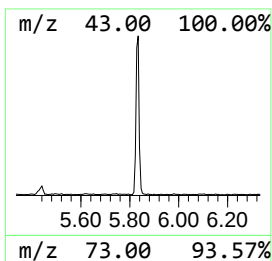
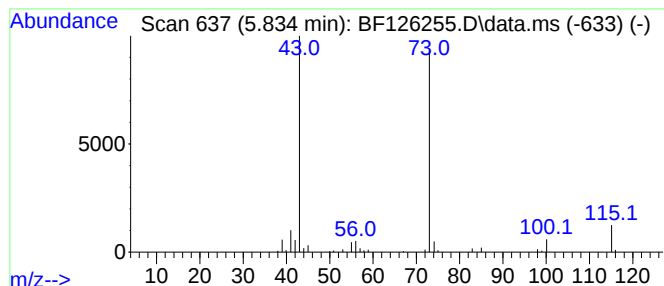
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	2.97 ng	202474	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10		
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9		
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	9		
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9		



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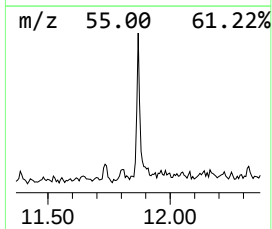
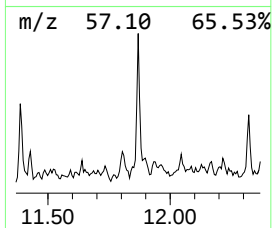
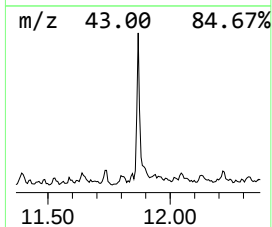
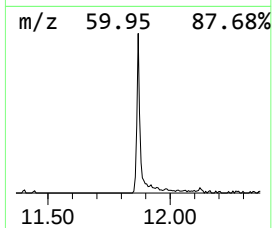
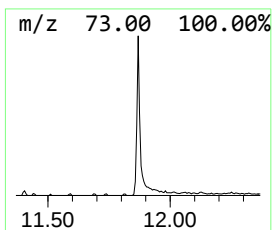
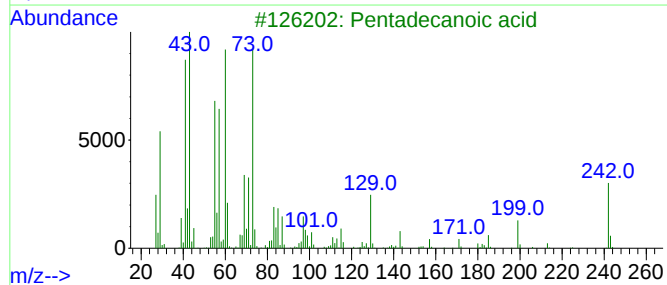
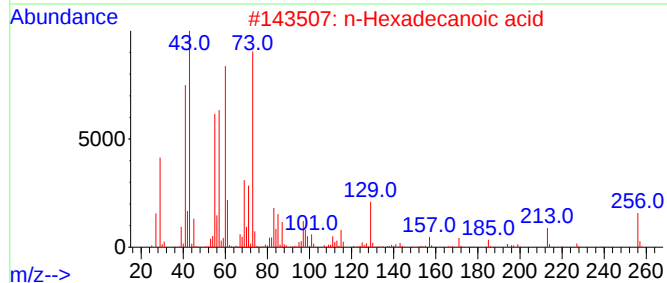
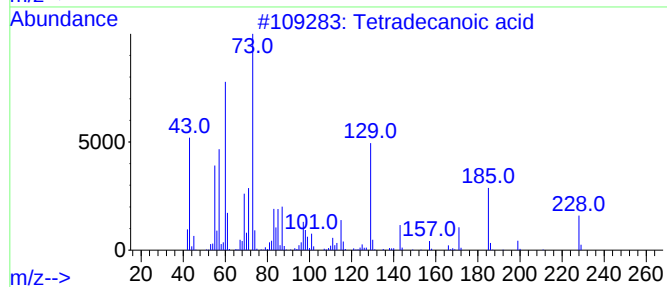
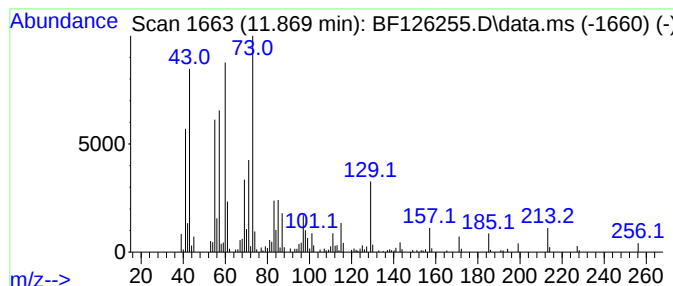
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	3.50 ng	351362	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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Acq On : 18 Dec 2021 15:39
Operator : JU/CG
Sample : M5082-02
Misc :
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Instrument :
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ClientSampleId :
SASP2-121-1(55-62)

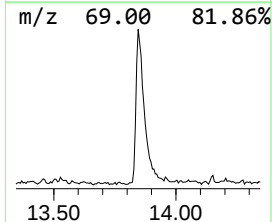
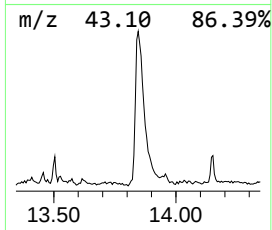
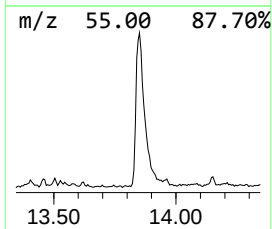
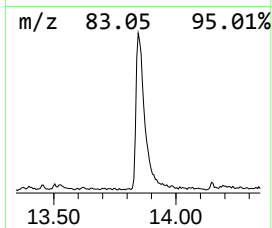
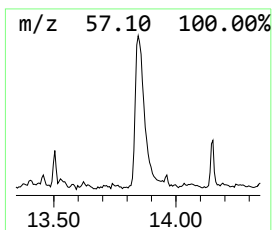
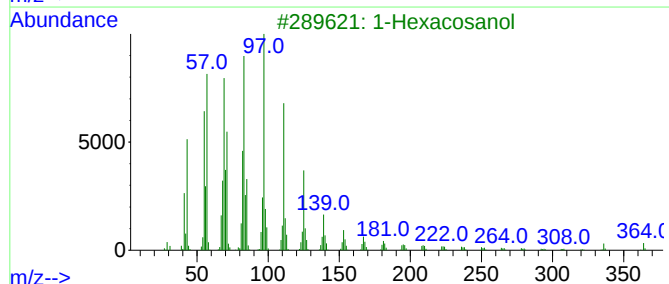
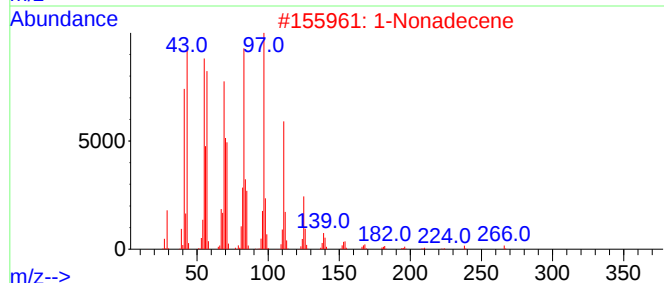
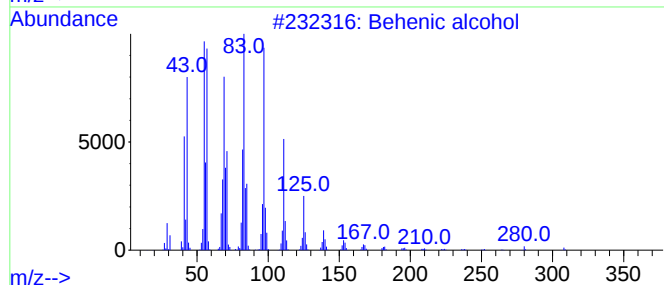
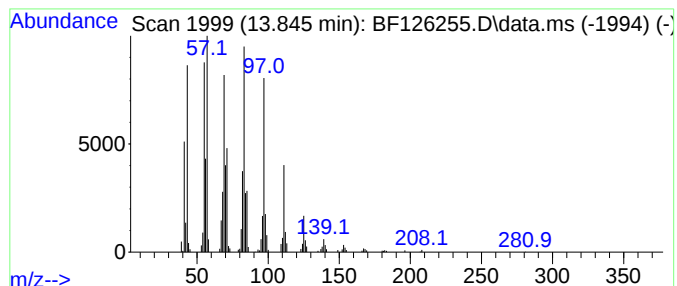
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	17.65 ng	1434250	Chrysene-d12	13.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		1-Hexacosanol	382	C26H54O	000506-52-5	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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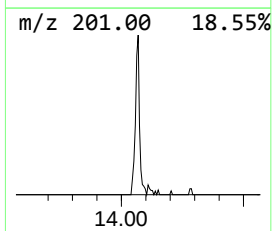
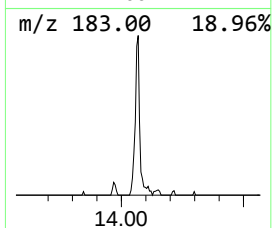
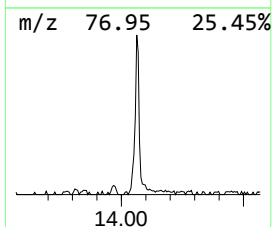
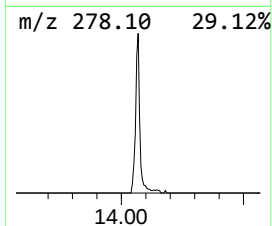
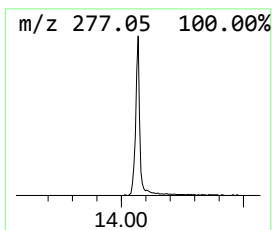
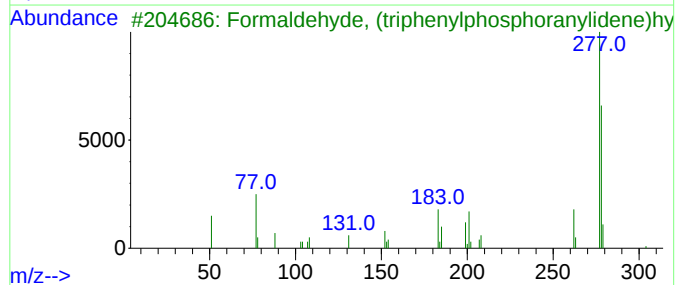
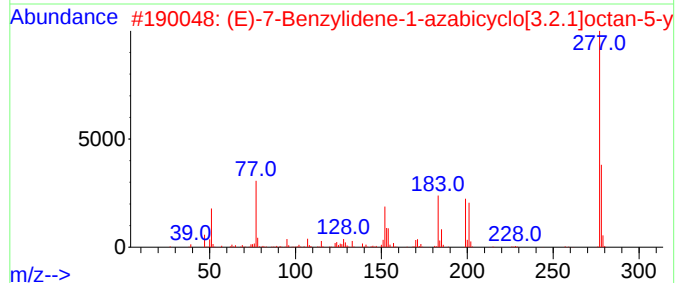
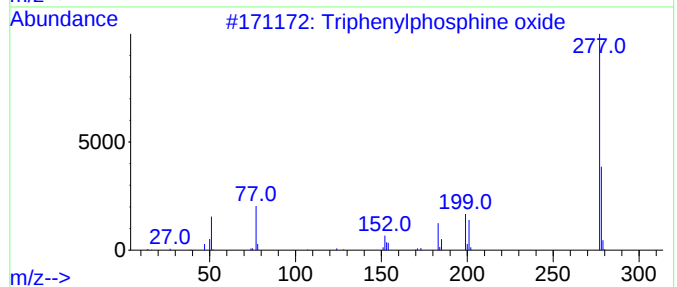
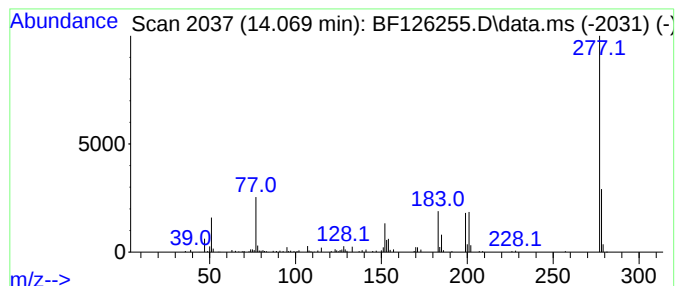
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.069	3.75 ng	304776	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	50
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47



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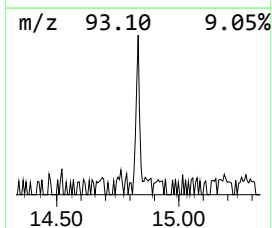
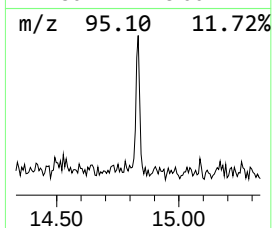
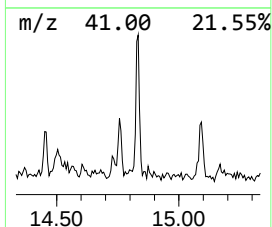
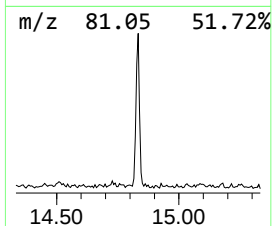
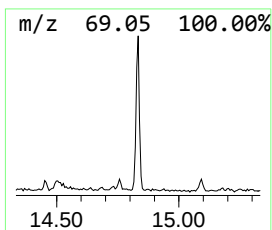
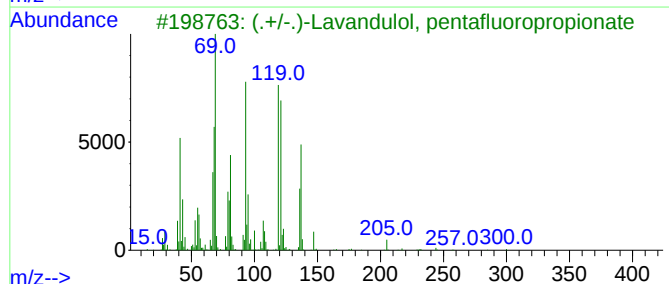
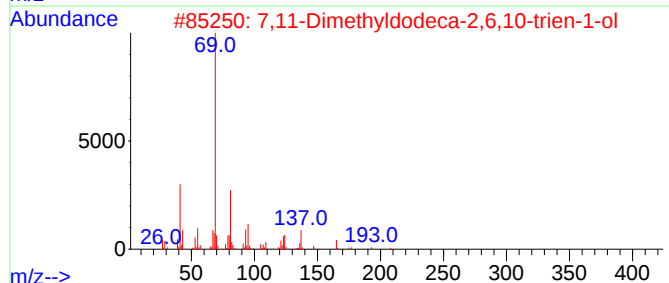
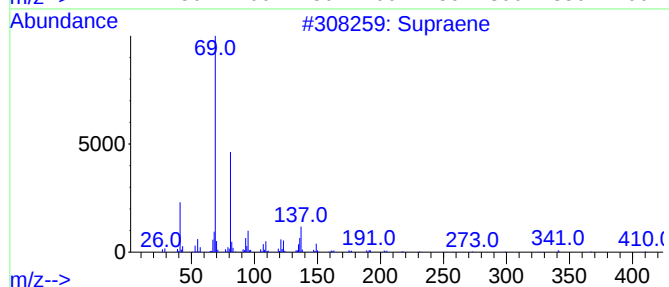
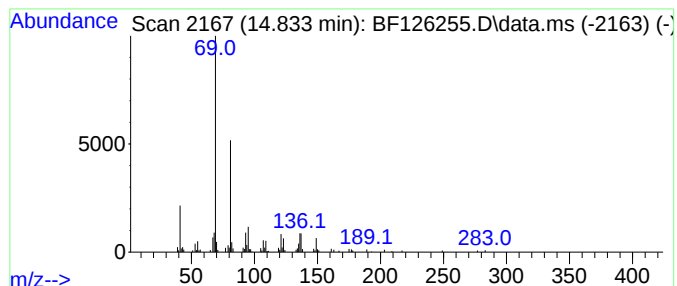
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.833	2.29 ng	151667	Perylene-d12		15.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72
3	(./-)-Lavandulol, pentafluorop...		300	C13H17F5O2	1000352-63-1	64
4	1,5-Heptadiene, 3,3,6-trimethyl-		138	C10H18	035387-63-4	58
5	2,3,5-Trimethyl-2,3,5-hexanetric...		203	C12H17N3	003974-79-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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Operator : JU/CG
Sample : M5082-02
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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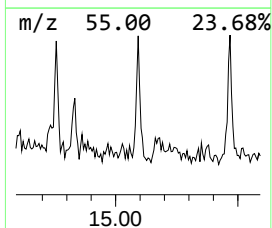
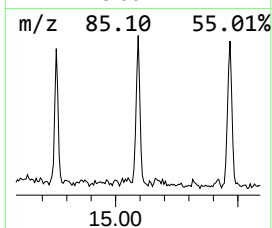
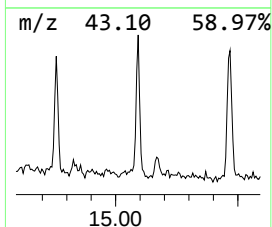
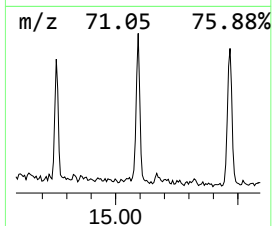
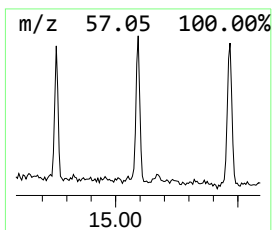
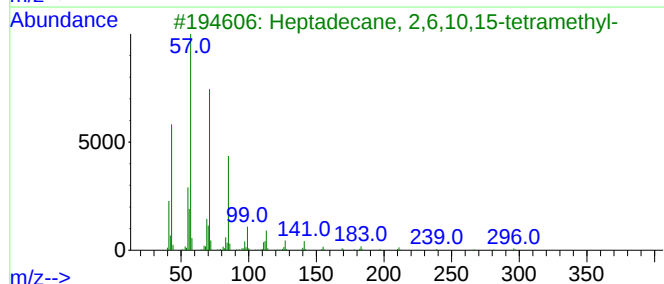
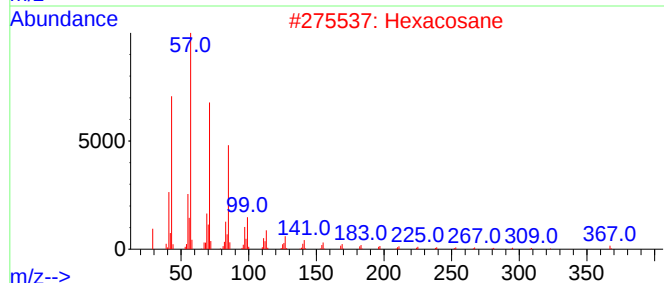
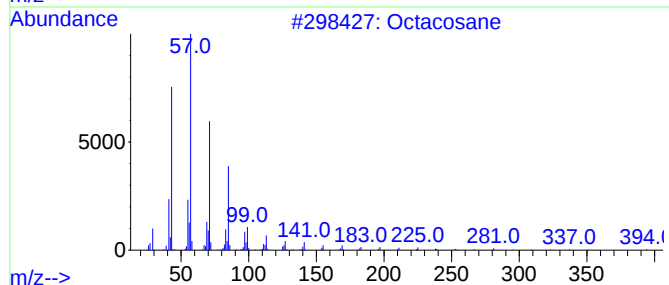
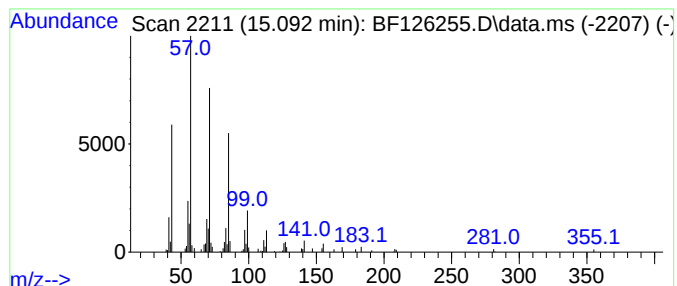
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.08 ng	137737	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Hexacosane	366	C26H54	000630-01-3	83
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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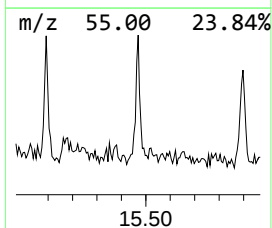
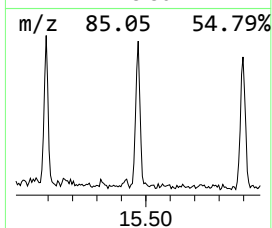
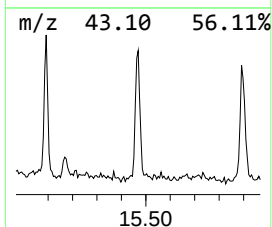
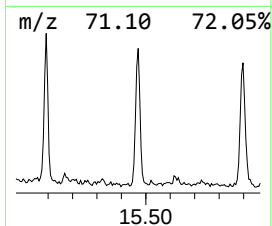
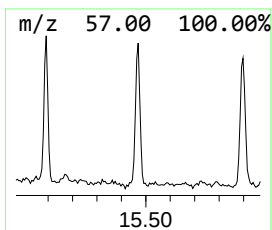
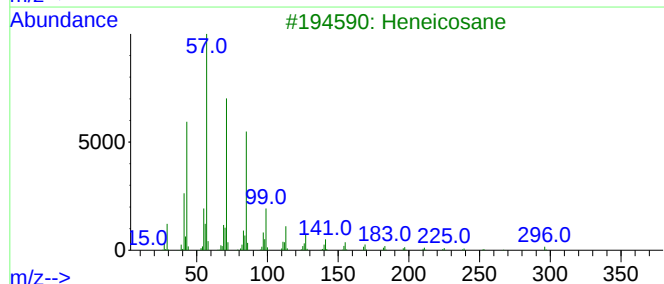
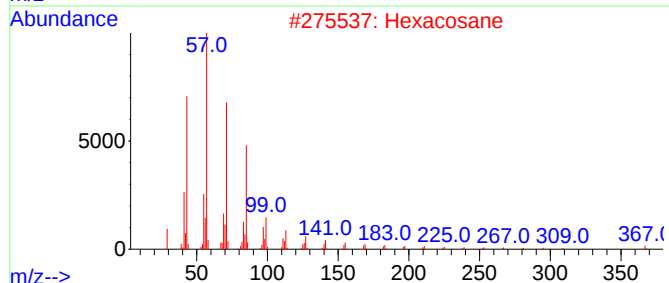
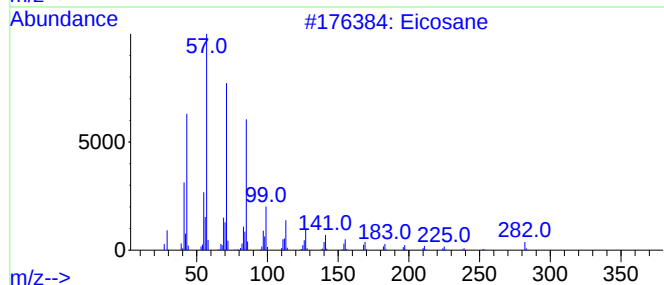
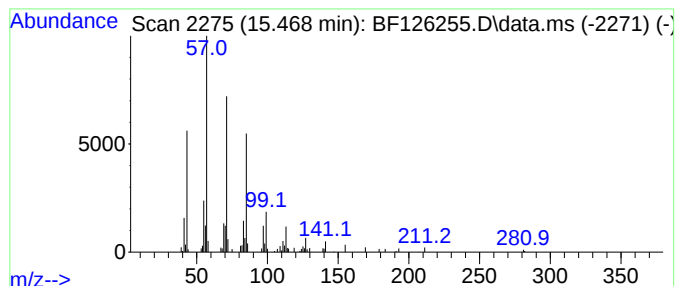
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	2.44 ng	161138	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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Operator : JU/CG
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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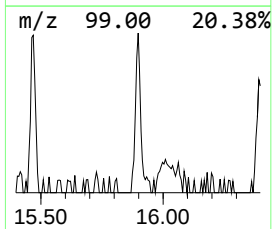
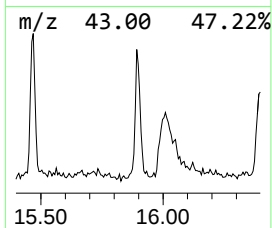
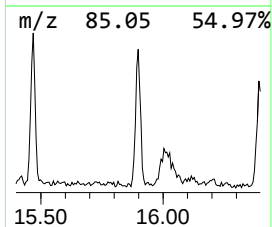
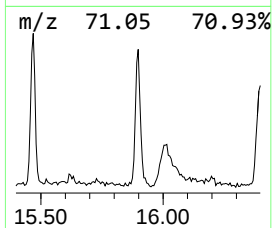
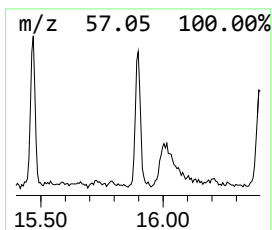
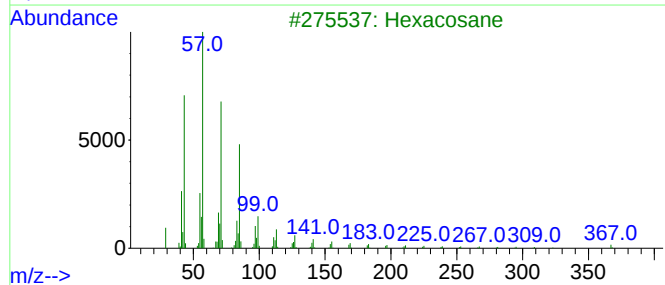
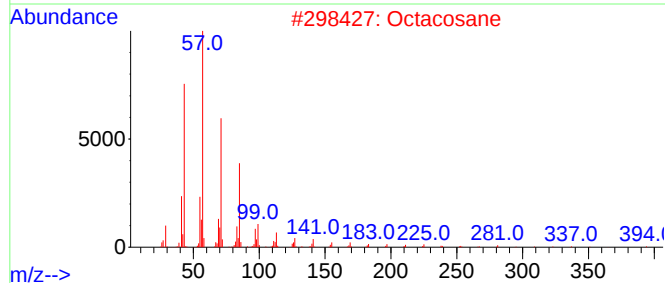
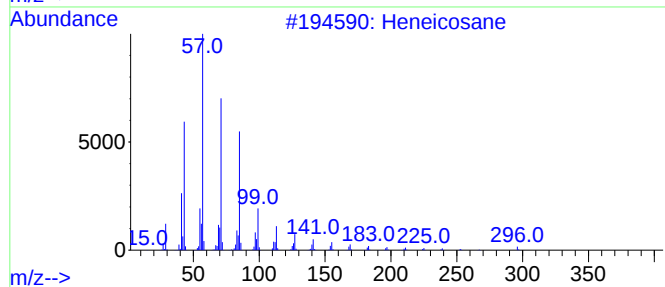
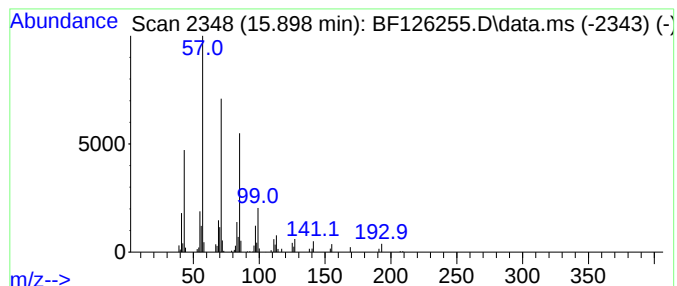
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.40 ng	158677	Perylene-d12	15.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	87
2		Octacosane	394	C28H58	000630-02-4	83
3		Hexacosane	366	C26H54	000630-01-3	74
4		Tetracosane	338	C24H50	000646-31-1	72
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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Acq On : 18 Dec 2021 15:39
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Sample : M5082-02
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ALS Vial : 9 Sample Multiplier: 1

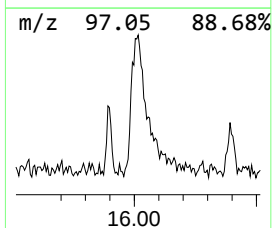
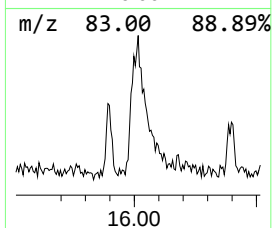
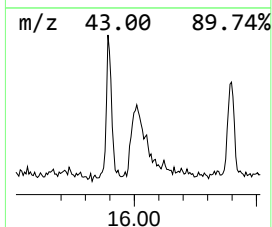
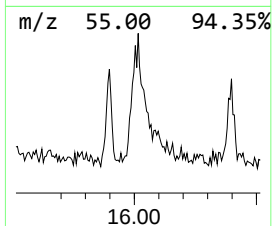
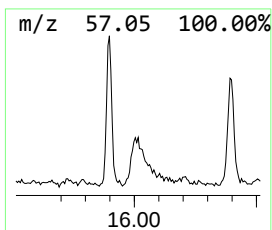
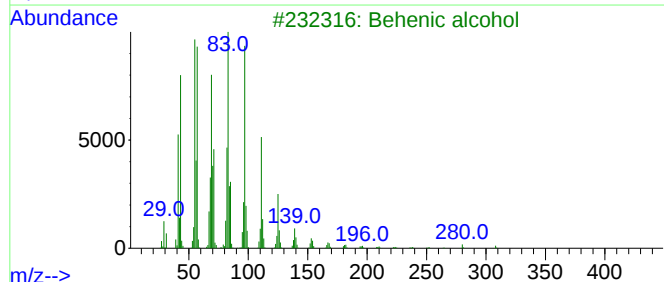
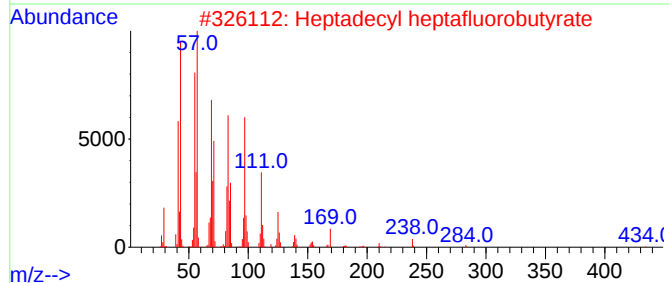
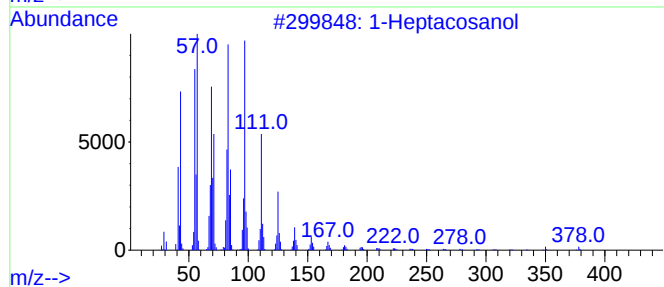
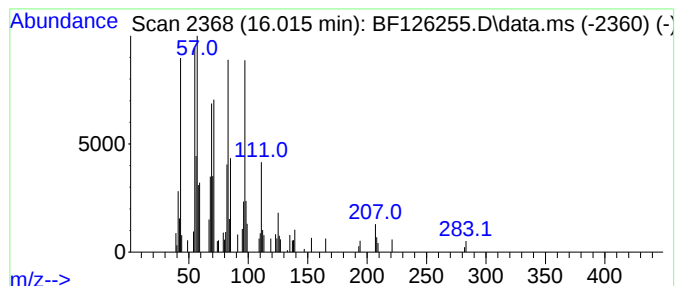
Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.015	4.39 ng	290205	Perylene-d12	15.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	1-Docosene	308	C22H44	001599-67-3	87
5	Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126255.D
Acq On : 18 Dec 2021 15:39
Operator : JU/CG
Sample : M5082-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

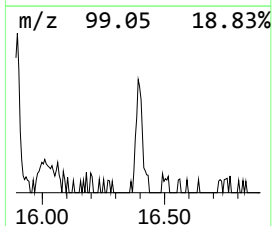
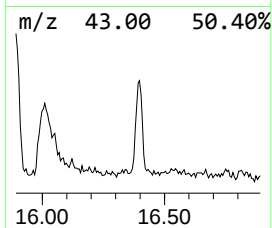
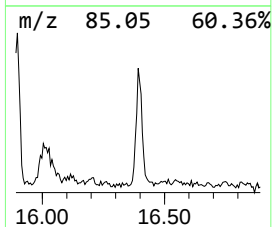
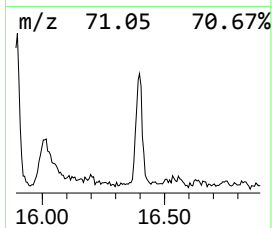
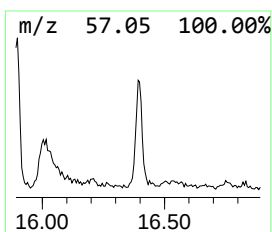
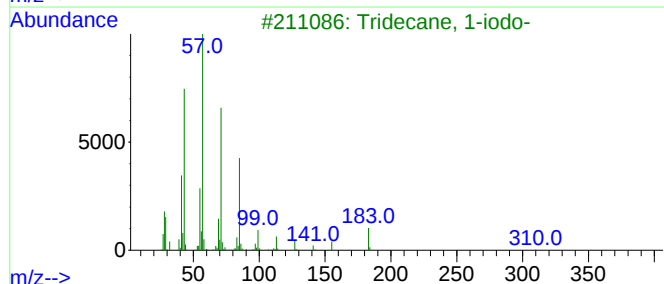
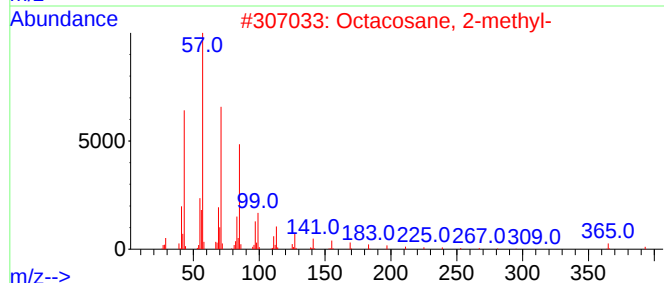
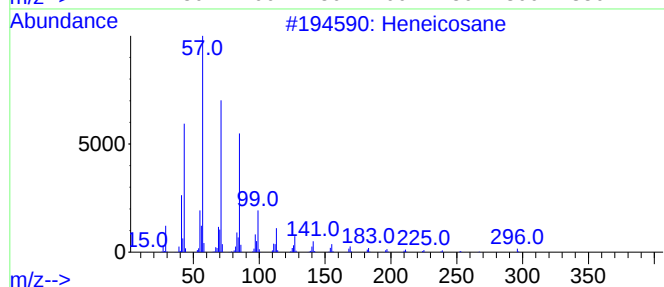
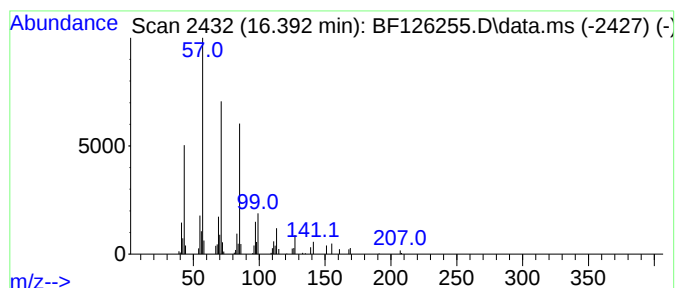
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	2.39 ng	157792	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86
5			Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126255.D
Acq On : 18 Dec 2021 15:39
Operator : JU/CG
Sample : M5082-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	17.3	ng	1181890	1	6.816	1364470	20.0
Propane, 1,1-di...	2.252	2.3	ng	154002	1	6.816	1364470	20.0
2-Pentanone, 4-...	5.040	28.1	ng	1920810	1	6.816	1364470	20.0
2-Pentanone, 4-...	5.834	3.0	ng	202474	1	6.816	1364470	20.0
Tetradecanoic acid	11.869	3.5	ng	351362	4	11.333	2009490	20.0
Behenic alcohol	13.845	17.6	ng	1434250	5	13.974	1625260	20.0
Triphenylphosph...	14.069	3.8	ng	304776	5	13.974	1625260	20.0
Supraene	14.833	2.3	ng	151667	6	15.416	1321950	20.0
Octacosane	15.092	2.1	ng	137737	6	15.416	1321950	20.0
Eicosane	15.469	2.4	ng	161138	6	15.416	1321950	20.0
Heneicosane	15.898	2.4	ng	158677	6	15.416	1321950	20.0
1-Heptacosanol	16.015	4.4	ng	290205	6	15.416	1321950	20.0
Octacosane, 2-m...	16.392	2.4	ng	157792	6	15.416	1321950	20.0