

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
 Data File : BF125322.D
 Acq On : 2 Sep 2021 15:55
 Operator : JU/CG
 Sample : M3606-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BPU-1

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125322.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	31	rVB	2951462	4031630	58.51%	10.569%
2	5.528	580	585	588	rBV	2188075	2143374	31.11%	5.619%
3	6.533	752	756	769	rVB	1490520	1334183	19.36%	3.498%
4	6.904	816	819	823	rBV	1064956	934843	13.57%	2.451%
5	7.475	910	916	919	rBV	3352512	3150584	45.72%	8.260%
6	8.098	1018	1022	1034	rBV	225685	428603	6.22%	1.124%
7	8.192	1034	1038	1041	rBV	1535650	1213120	17.61%	3.180%
8	9.269	1216	1221	1224	rBV	6029434	5426355	78.75%	14.226%
9	9.951	1333	1337	1340	rBV	1554932	1436331	20.84%	3.765%
10	10.139	1365	1369	1377	rBV2	47292	80185	1.16%	0.210%
11	10.739	1467	1471	1475	rBV	3722592	3918260	56.86%	10.272%
12	11.439	1586	1590	1593	rBV	1851932	1588583	23.05%	4.165%
13	11.951	1672	1677	1683	rBV	436061	541360	7.86%	1.419%
14	12.739	1806	1811	1820	rVB	234548	301784	4.38%	0.791%
15	13.027	1848	1860	1863	rBV	6305747	6890731	100.00%	18.065%
16	13.827	1988	1996	2001	rBV	173157	329940	4.79%	0.865%
17	13.909	2006	2010	2013	rBV2	59715	78789	1.14%	0.207%
18	13.945	2013	2016	2022	rBV	185987	220938	3.21%	0.579%
19	14.080	2035	2039	2043	rBV	1625061	1451115	21.06%	3.804%
20	14.457	2096	2103	2108	rBV	158109	336994	4.89%	0.883%
21	14.515	2109	2113	2115	rBV2	72662	111550	1.62%	0.292%
22	15.033	2196	2201	2208	rBV	120267	220147	3.19%	0.577%
23	15.204	2226	2230	2236	rVB	75604	91694	1.33%	0.240%
24	15.586	2289	2295	2304	rBV	1007375	1370390	19.89%	3.593%
25	15.698	2308	2314	2322	rVB2	98684	224055	3.25%	0.587%
26	16.045	2369	2373	2378	rVB	78469	100364	1.46%	0.263%
27	16.898	2513	2518	2527	rVB4	82480	188598	2.74%	0.494%

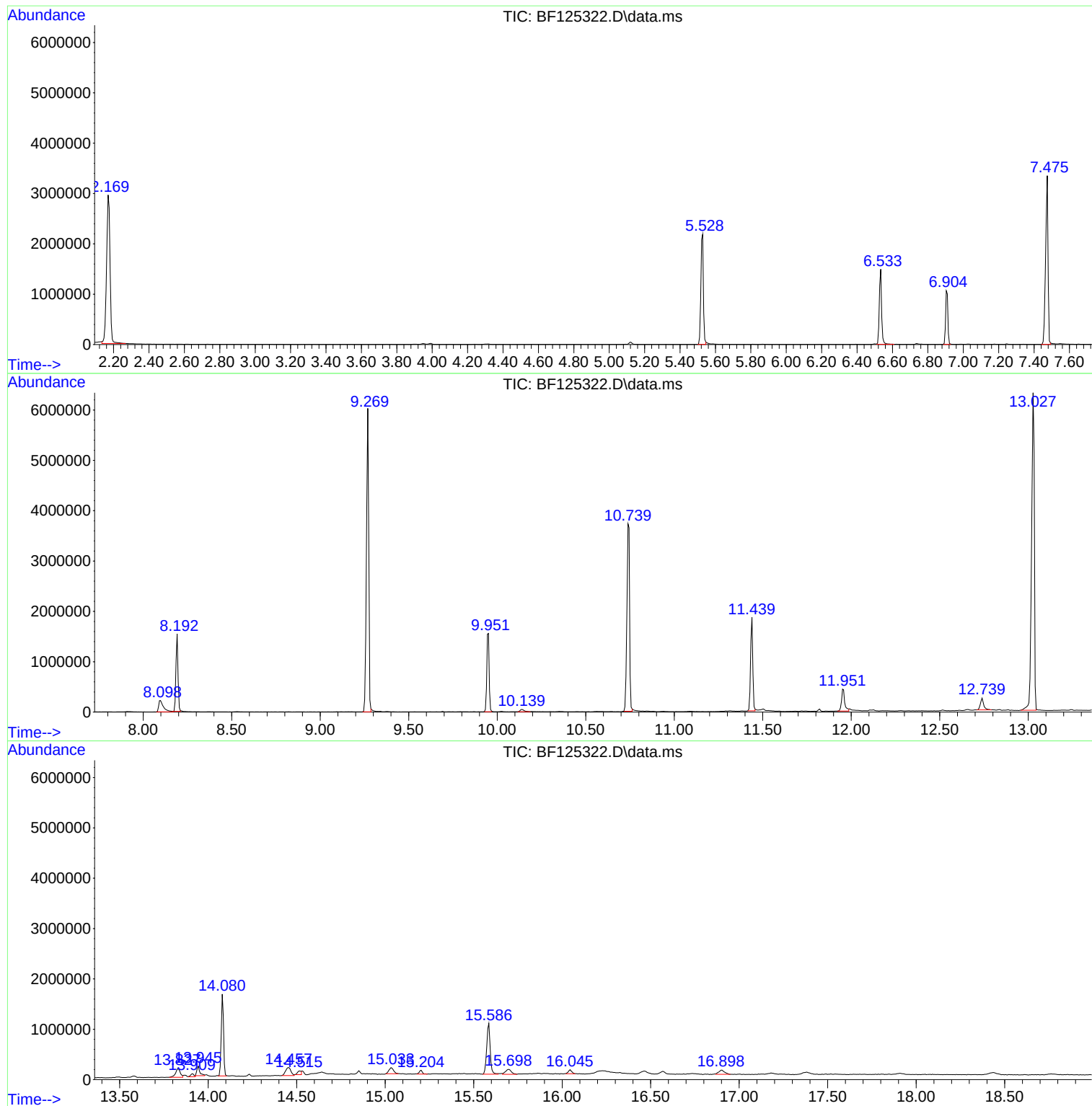
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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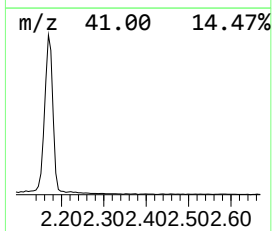
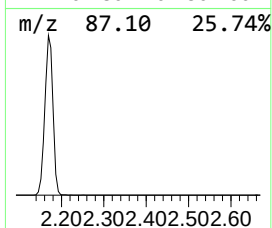
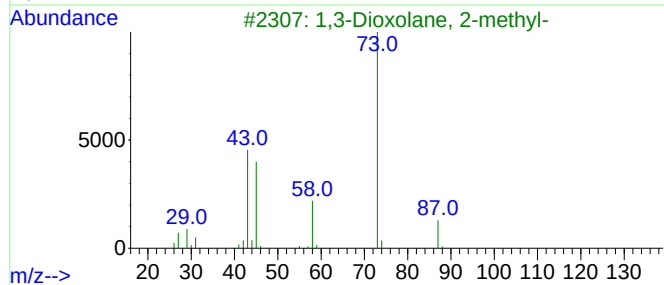
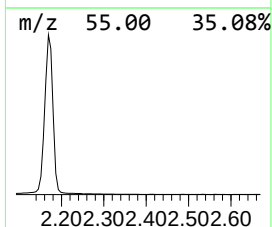
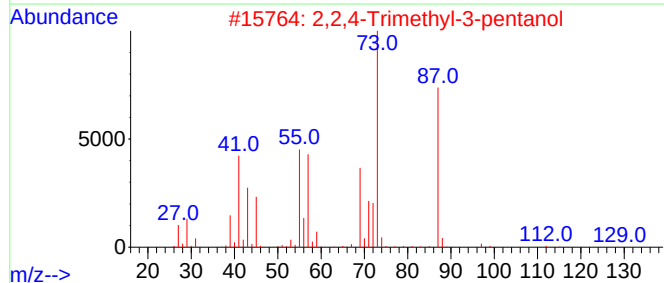
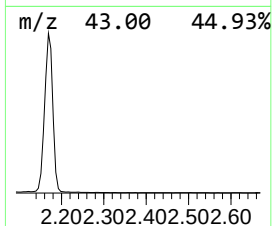
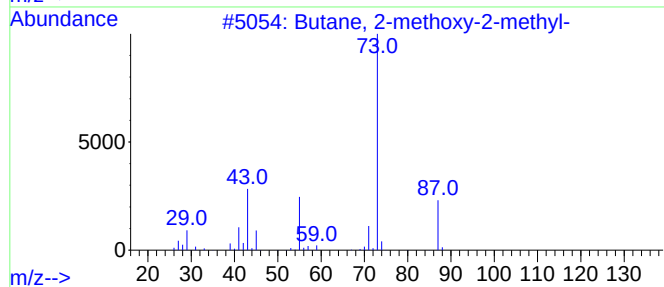
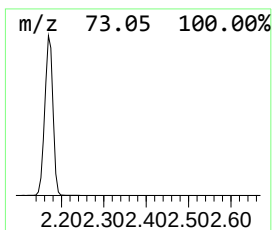
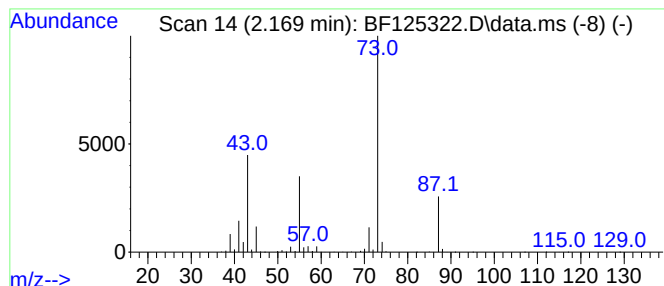
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	86.25 ng	4031630	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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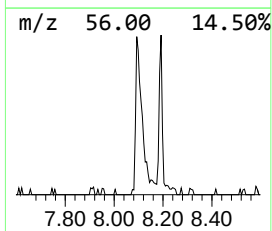
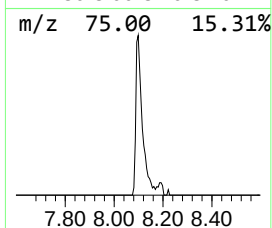
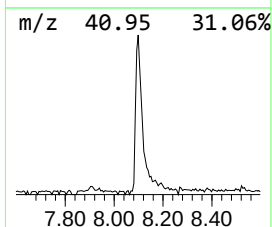
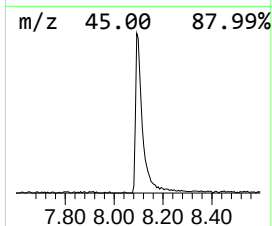
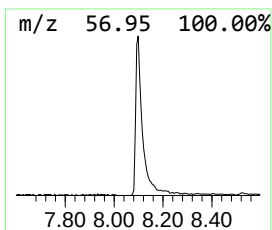
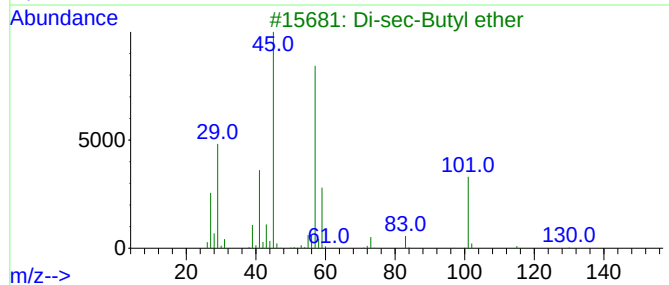
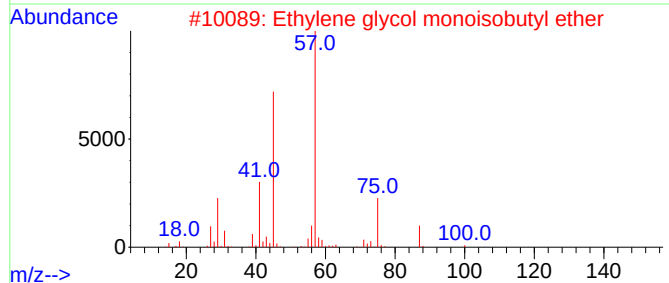
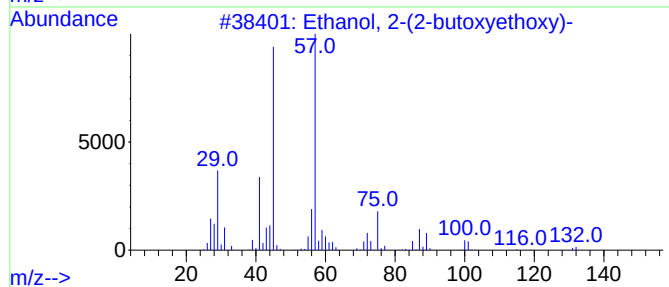
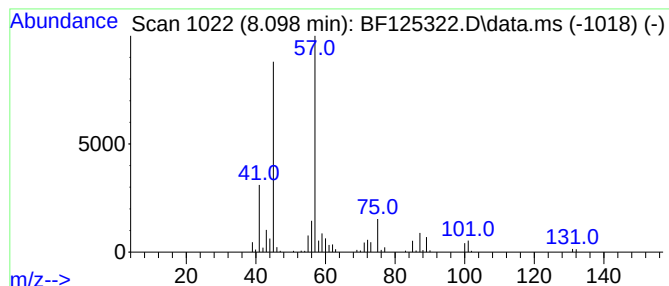
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	7.07 ng	428603	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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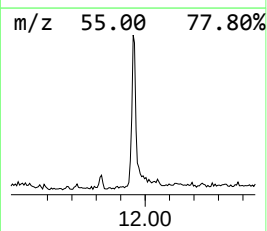
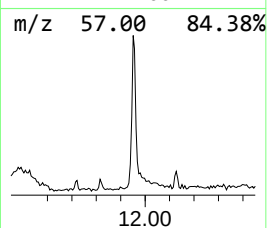
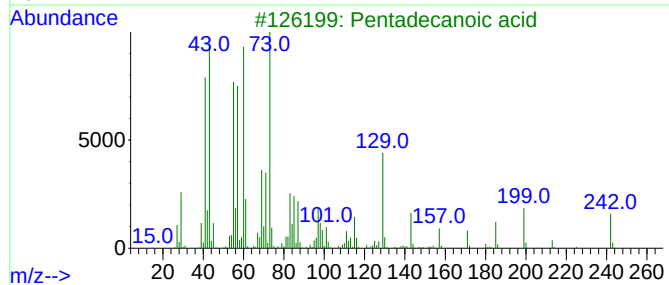
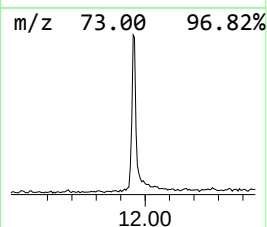
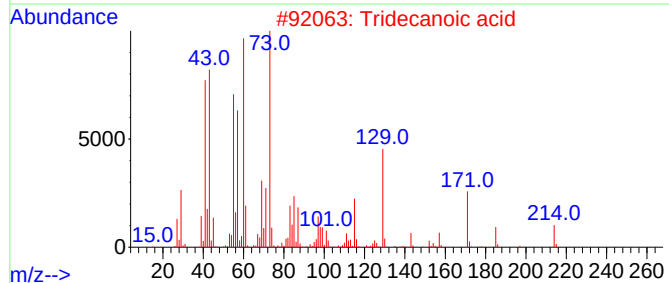
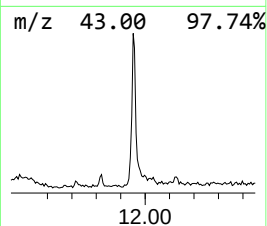
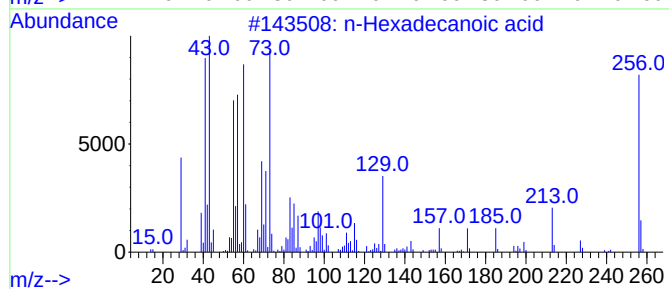
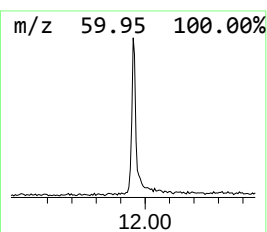
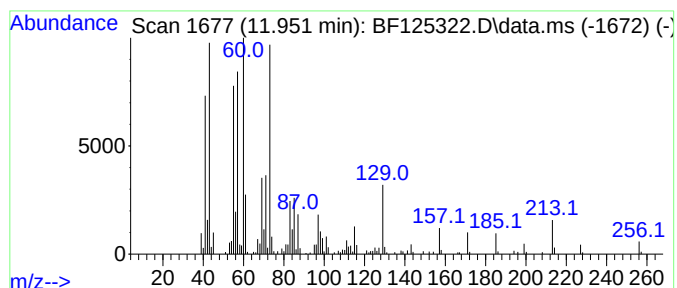
Instrument :
BNA_F
ClientSampleId :
BPU-1

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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.951	6.82 ng	541360	Phenanthrene-d10	11.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-1

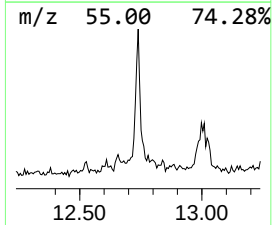
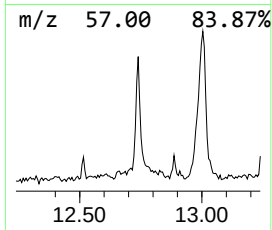
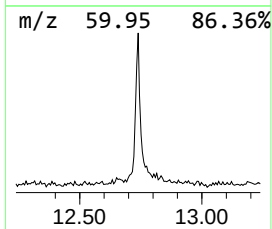
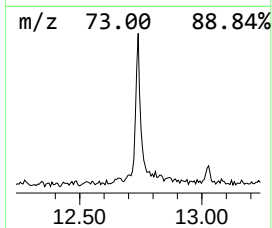
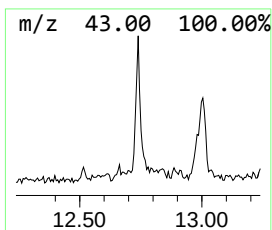
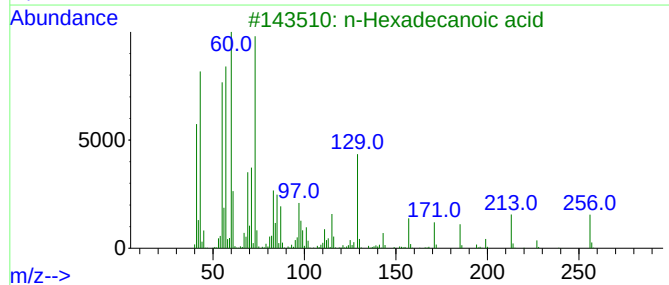
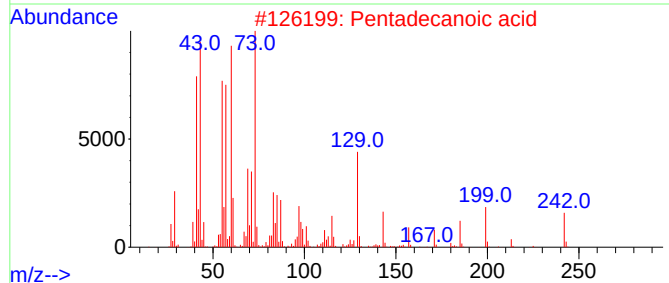
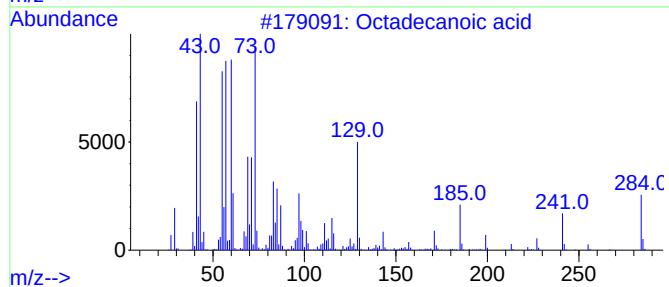
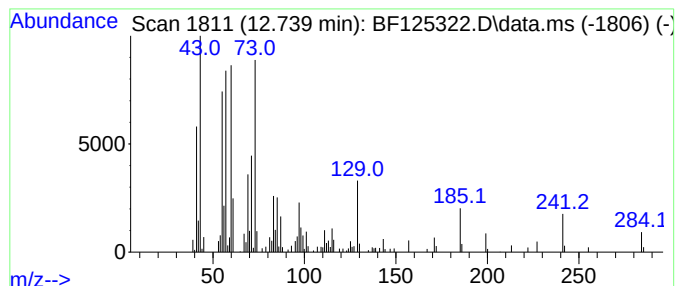
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	3.80 ng	301784	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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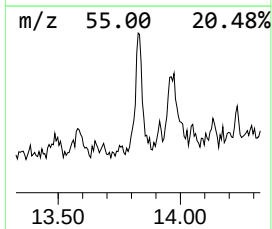
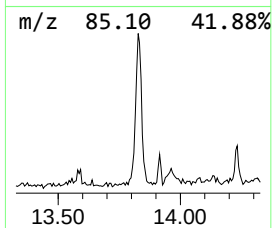
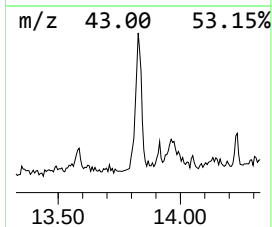
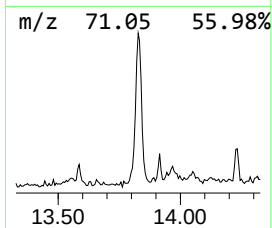
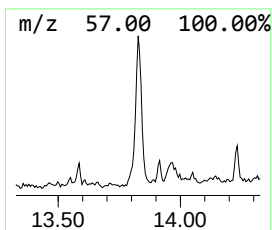
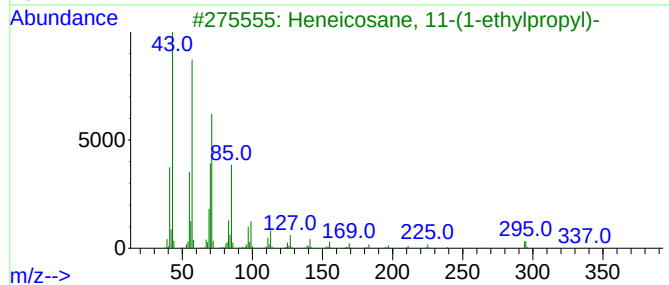
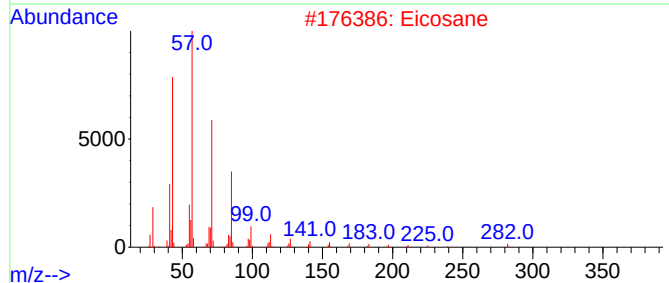
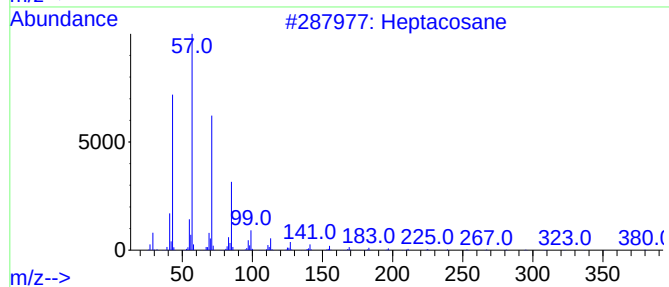
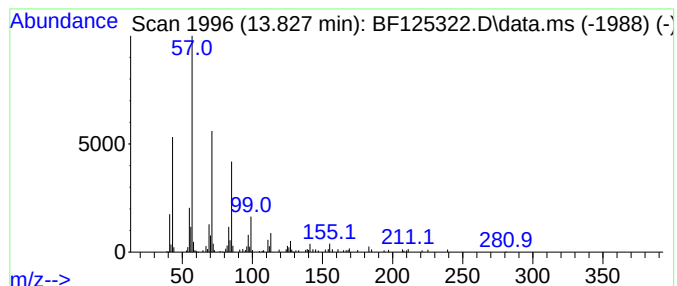
Instrument :
BNA_F
ClientSampled :
BPU-1

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Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.827	4.55 ng	329940	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90



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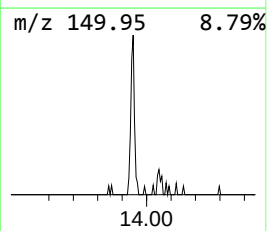
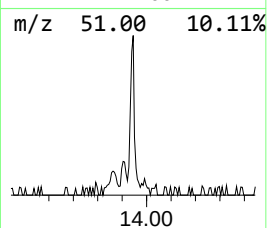
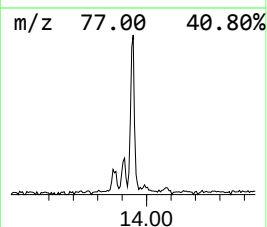
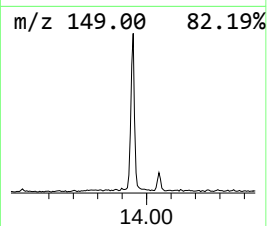
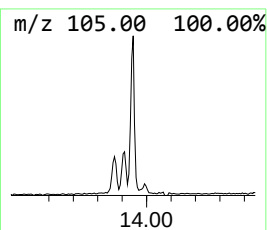
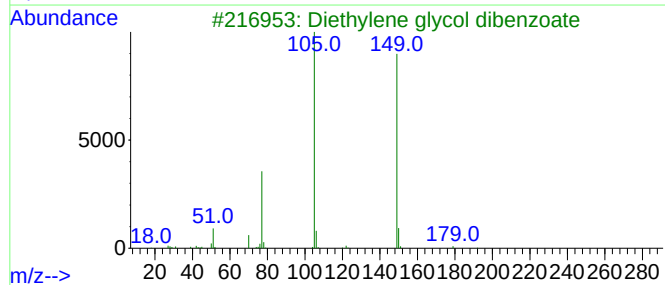
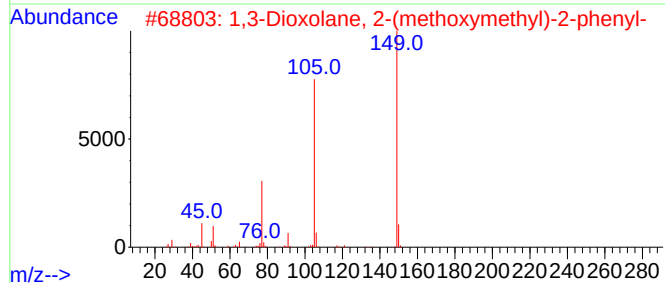
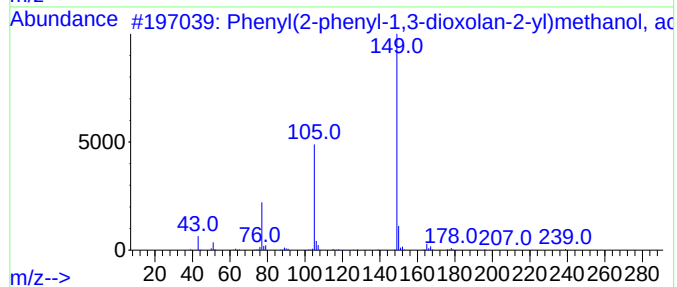
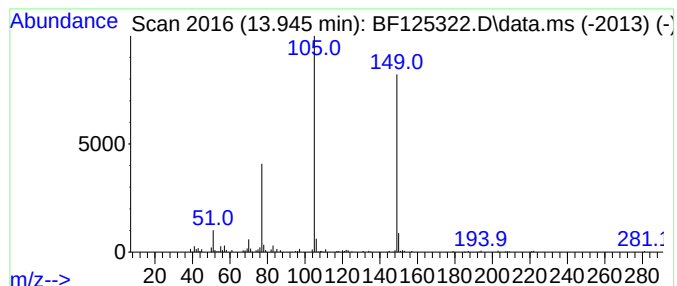
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	3.05 ng	220938	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
4			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
5			Phthalic acid, cycloheptyl hexyl...	346	C21H30O4	1000322-83-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125322.D
Acq On : 2 Sep 2021 15:55
Operator : JU/CG
Sample : M3606-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BPU-1

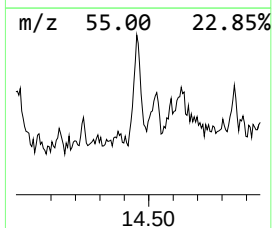
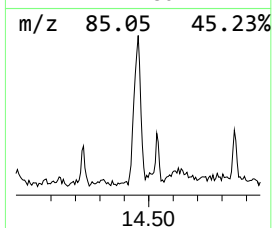
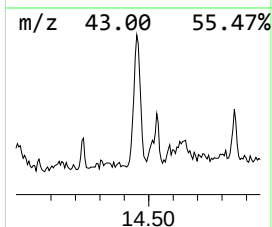
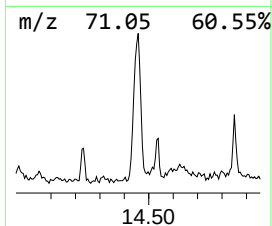
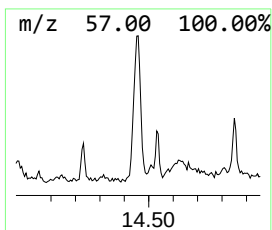
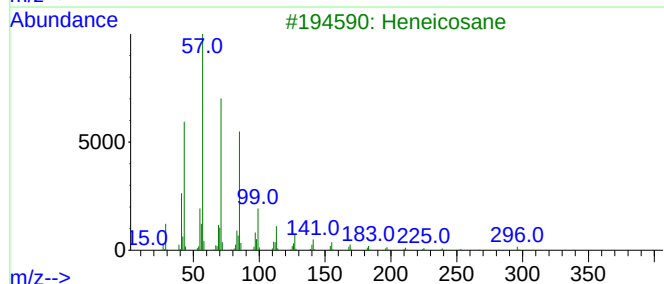
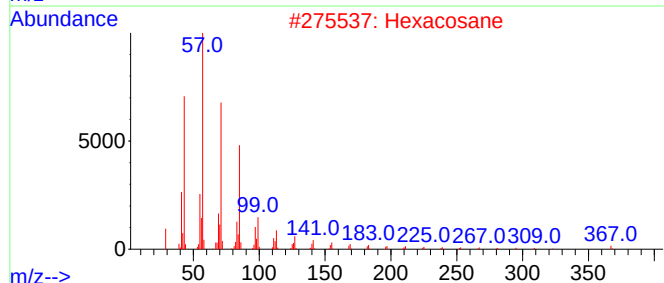
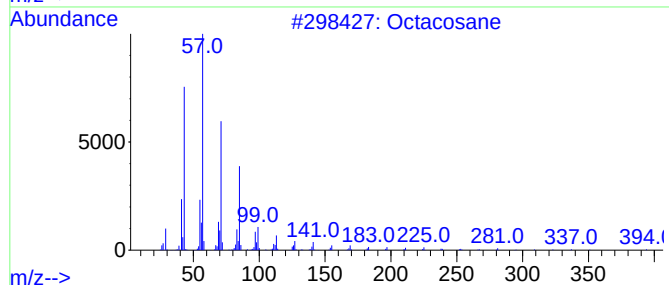
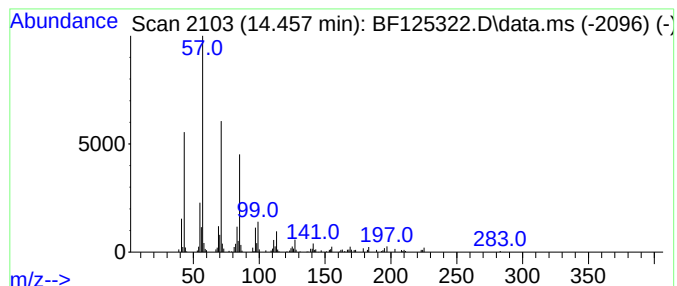
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	4.64 ng	336994	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Docosane	310	C22H46	000629-97-0	87
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125322.D
Acq On : 2 Sep 2021 15:55
Operator : JU/CG
Sample : M3606-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BPU-1

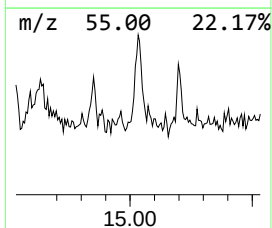
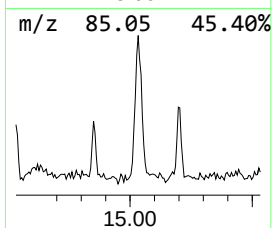
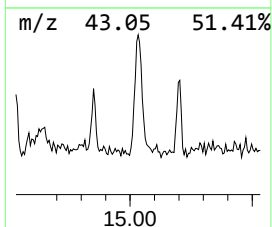
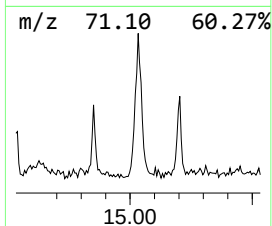
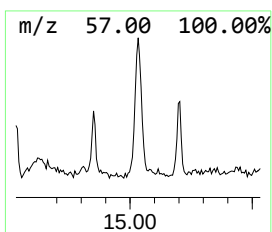
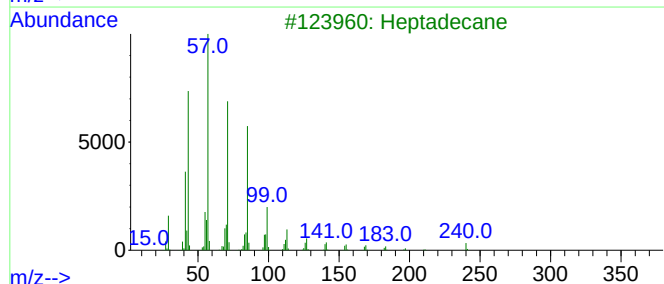
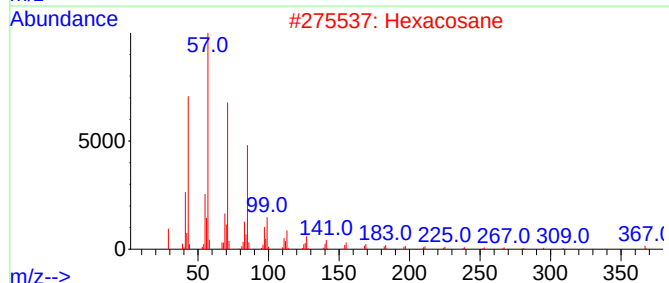
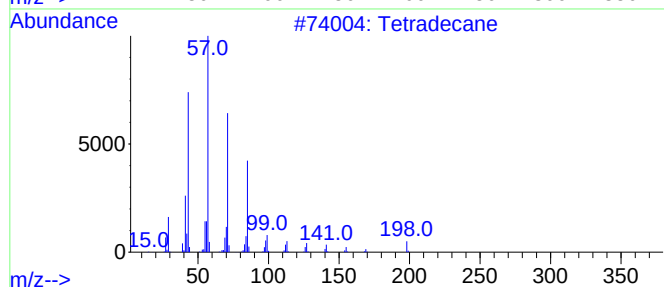
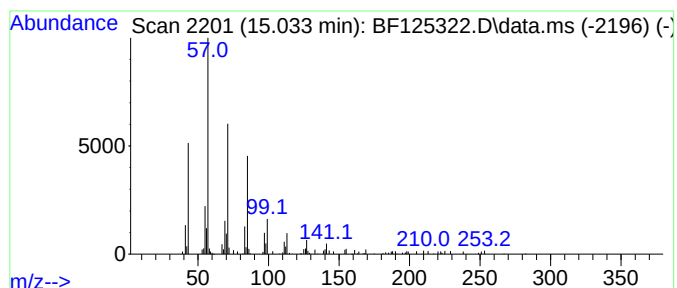
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	3.21 ng	220147	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Hexacosane	366	C26H54	000630-01-3	87
3			Heptadecane	240	C17H36	000629-78-7	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Hexatriacontane	507	C36H74	000630-06-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125322.D
Acq On : 2 Sep 2021 15:55
Operator : JU/CG
Sample : M3606-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-1

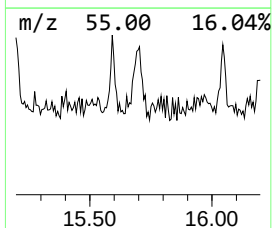
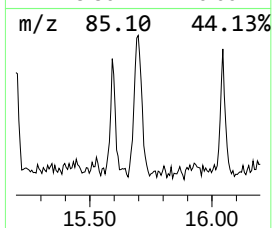
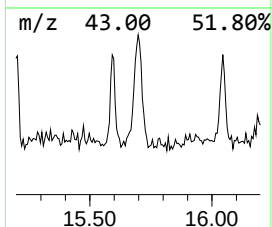
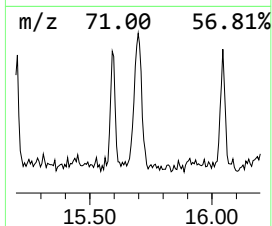
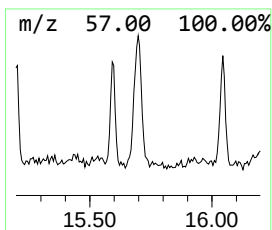
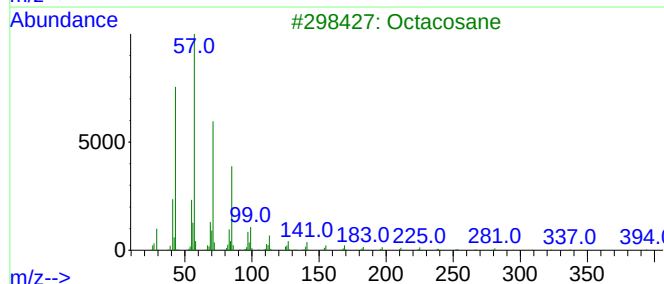
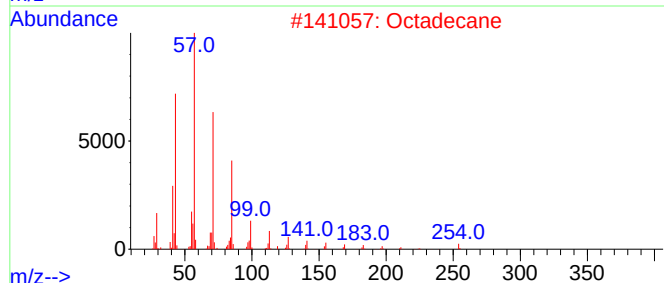
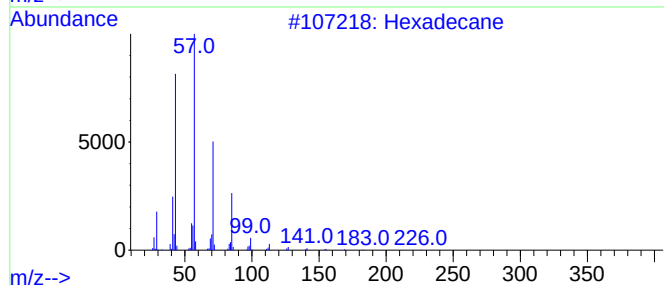
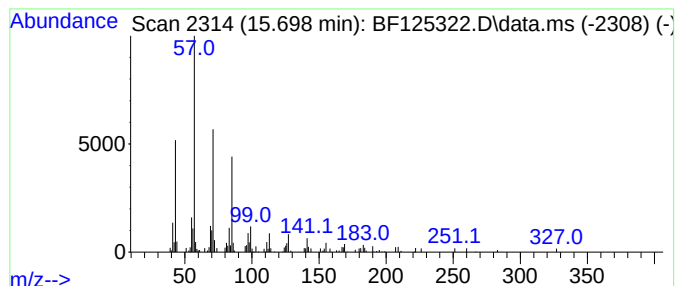
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	3.27 ng	224055	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane			226	C16H34	000544-76-3	91
2	Octadecane			254	C18H38	000593-45-3	86
3	Octacosane			394	C28H58	000630-02-4	86
4	Heneicosane			296	C21H44	000629-94-7	86
5	Hexacosane			366	C26H54	000630-01-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125322.D
Acq On : 2 Sep 2021 15:55
Operator : JU/CG
Sample : M3606-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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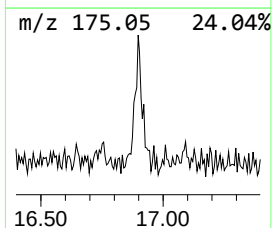
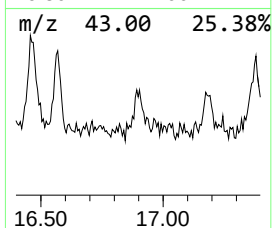
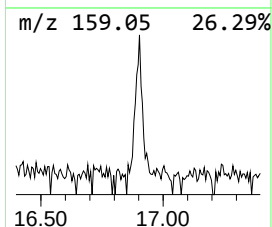
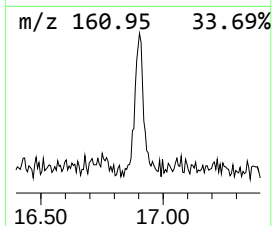
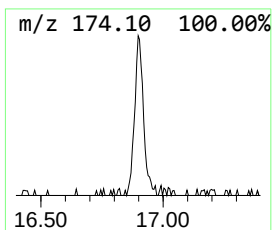
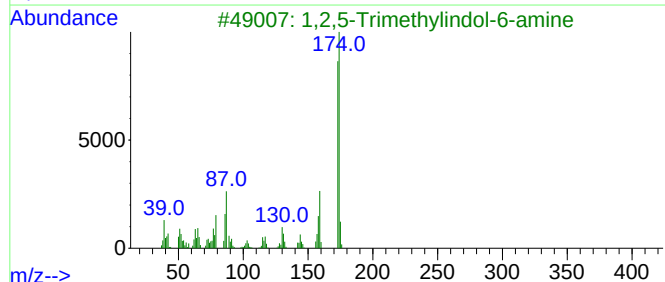
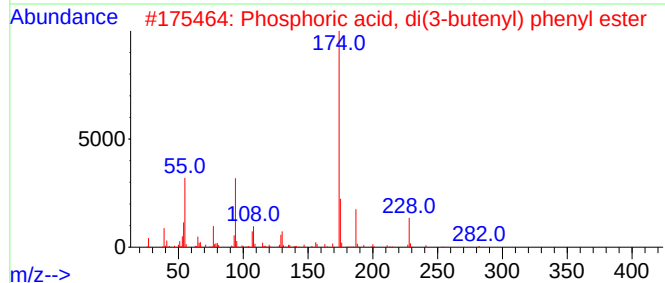
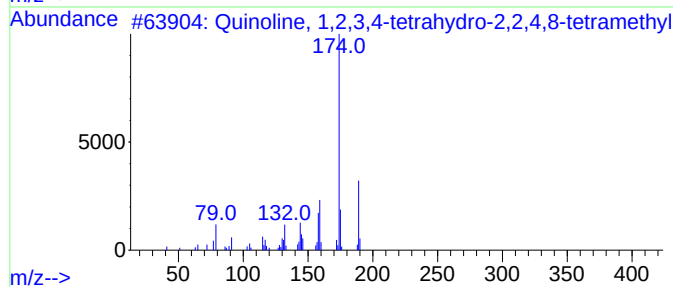
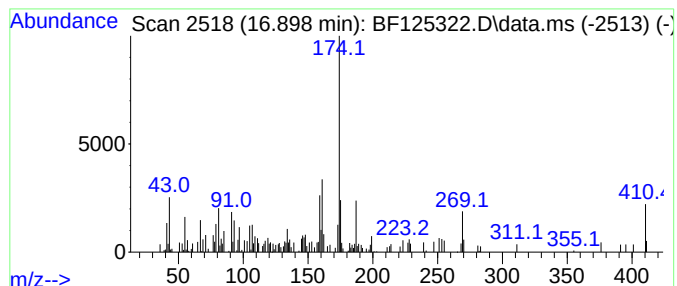
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.898 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	2.75 ng	188598	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 1,2,3,4-tetrahydro-2,...	189	C13H19N	1000308-78-8	47		
2	Phosphoric acid, di(3-butenyl) p...	282	C14H19O4P	006612-66-4	47		
3	1,2,5-Trimethylindol-6-amine	174	C11H14N2	1000389-10-0	43		
4	7-Methoxy-1-naphthol	174	C11H10O2	067247-13-6	43		
5	4-Ethynylaniline, N-(tert-butyld...	231	C14H21NSi	1000449-79-1	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125322.D
Acq On : 2 Sep 2021 15:55
Operator : JU/CG
Sample : M3606-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.169	86.3	ng	4031630	1	6.910	934843	20.0
Ethanol, 2-(2-b...	8.098	7.1	ng	428603	2	8.192	1213120	20.0
n-Hexadecanoic ...	11.951	6.8	ng	541360	4	11.439	1588580	20.0
Octadecanoic acid	12.739	3.8	ng	301784	4	11.439	1588580	20.0
Heptacosane	13.827	4.5	ng	329940	5	14.080	1451120	20.0
Phenyl(2-phenyl...	13.945	3.0	ng	220938	5	14.080	1451120	20.0
Octacosane	14.457	4.6	ng	336994	5	14.080	1451120	20.0
Tetradecane	15.033	3.2	ng	220147	6	15.586	1370390	20.0
Hexadecane	15.698	3.3	ng	224055	6	15.586	1370390	20.0
unknown16.898	16.898	2.8	ng	188598	6	15.586	1370390	20.0