

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
 Data File : BF126381.D
 Acq On : 28 Dec 2021 15:01
 Operator : JU/CG
 Sample : M5187-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2-119-1-0-5

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: BF126381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.857	295	301	309	rVB	15890	22224	1.10%	0.136%
2	5.016	491	498	503	rBV	43951	55594	2.74%	0.341%
3	5.422	562	567	570	rBV	2131447	1975667	97.53%	12.126%
4	6.440	735	740	754	rBV	1929070	2025644	100.00%	12.433%
5	6.810	799	803	806	rBV	730963	578573	28.56%	3.551%
6	7.369	893	898	901	rBV	1454910	1283253	63.35%	7.876%
7	8.092	1017	1021	1024	rBV	891467	753712	37.21%	4.626%
8	9.169	1200	1204	1207	rBV	2250755	1881837	92.90%	11.550%
9	9.257	1215	1219	1224	rVB2	41496	43453	2.15%	0.267%
10	9.728	1292	1299	1306	rBV5	12398	31941	1.58%	0.196%
11	9.786	1306	1309	1312	rVB	28494	24918	1.23%	0.153%
12	9.845	1315	1319	1323	rBV	870228	746337	36.84%	4.581%
13	10.280	1391	1393	1396	rVB	24405	22000	1.09%	0.135%
14	10.633	1449	1453	1462	rBV	1143476	1006641	49.69%	6.178%
15	10.757	1472	1474	1483	rVB3	27248	43096	2.13%	0.265%
16	11.204	1543	1550	1553	rBV5	30905	44846	2.21%	0.275%
17	11.298	1562	1566	1568	rBV3	26444	22388	1.11%	0.137%
18	11.333	1568	1572	1574	rBV	735464	656528	32.41%	4.030%
19	11.351	1574	1575	1578	rVB	41122	31064	1.53%	0.191%
20	11.863	1655	1662	1666	rBV	219336	278601	13.75%	1.710%
21	12.316	1729	1739	1741	rBV3	38565	57241	2.83%	0.351%
22	12.374	1746	1749	1753	rVV4	47079	71062	3.51%	0.436%
23	12.416	1753	1756	1762	rVB7	15447	28667	1.42%	0.176%
24	12.545	1775	1778	1780	rBV	50638	49344	2.44%	0.303%
25	12.651	1791	1796	1806	rBV	297160	413065	20.39%	2.535%
26	12.769	1814	1816	1820	rVB	49551	46274	2.28%	0.284%
27	12.921	1838	1842	1845	rVB	1578700	1408083	69.51%	8.642%
28	13.398	1919	1923	1927	rVB4	20088	28384	1.40%	0.174%
29	13.492	1930	1939	1945	rBV2	64026	163954	8.09%	1.006%
30	13.845	1989	1999	2000	rBV4	34768	75743	3.74%	0.465%
31	13.868	2000	2003	2015	rVV3	89183	237384	11.72%	1.457%
32	13.968	2016	2020	2023	rVV	638062	646916	31.94%	3.971%
33	13.992	2023	2024	2032	rVB	105174	94280	4.65%	0.579%
34	14.145	2047	2050	2056	rVB	27513	25742	1.27%	0.158%
35	14.216	2056	2062	2067	rBV2	102179	184029	9.08%	1.130%
36	14.263	2067	2070	2075	rVB6	23815	35340	1.74%	0.217%

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37	14.451	2099	2102	2105	rVB	48826	49152	2.43%	0.302%
38	14.751	2150	2153	2157	rVV	49835	49009	2.42%	0.301%
39	14.810	2157	2163	2173	rVB4	62930	146347	7.22%	0.898%
40	14.998	2192	2195	2198	rBV2	23674	31470	1.55%	0.193%
41	15.086	2206	2210	2219	rVB2	64977	86309	4.26%	0.530%
42	15.292	2243	2245	2250	rVB	18407	21892	1.08%	0.134%
43	15.357	2252	2256	2261	rBV	20118	27105	1.34%	0.166%
44	15.421	2262	2267	2272	rBV	425348	592368	29.24%	3.636%
45	15.892	2343	2347	2350	rBV2	34874	59742	2.95%	0.367%
46	16.386	2426	2431	2442	rVB5	30571	71880	3.55%	0.441%
47	16.551	2453	2459	2468	rVB8	24332	63725	3.15%	0.391%

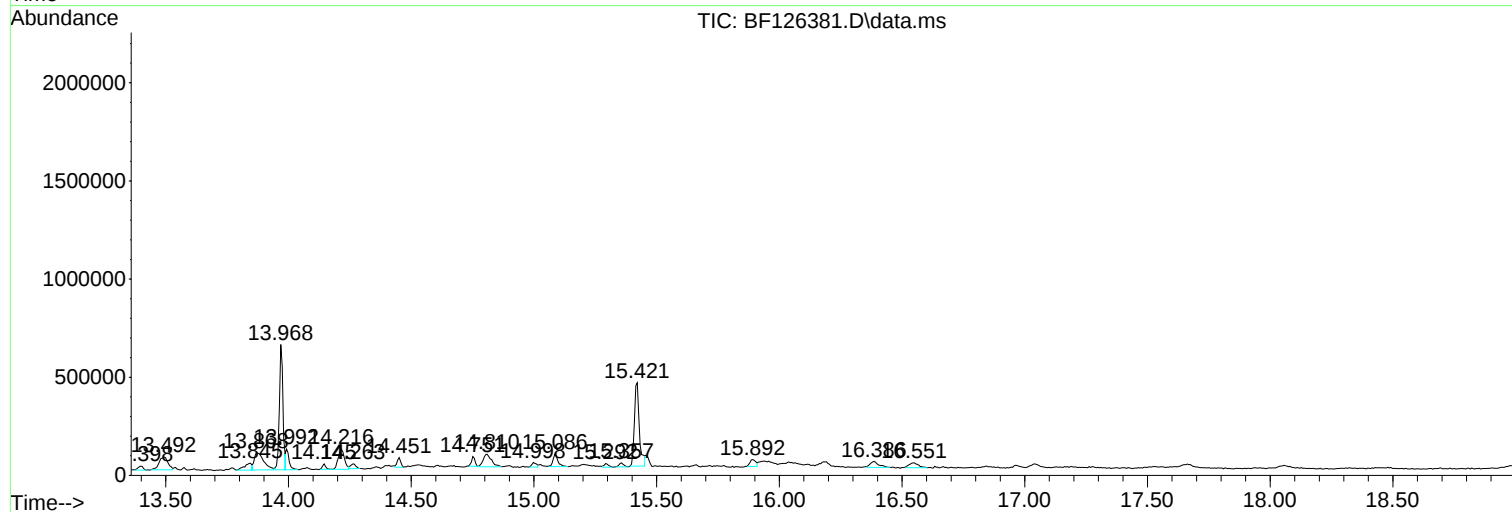
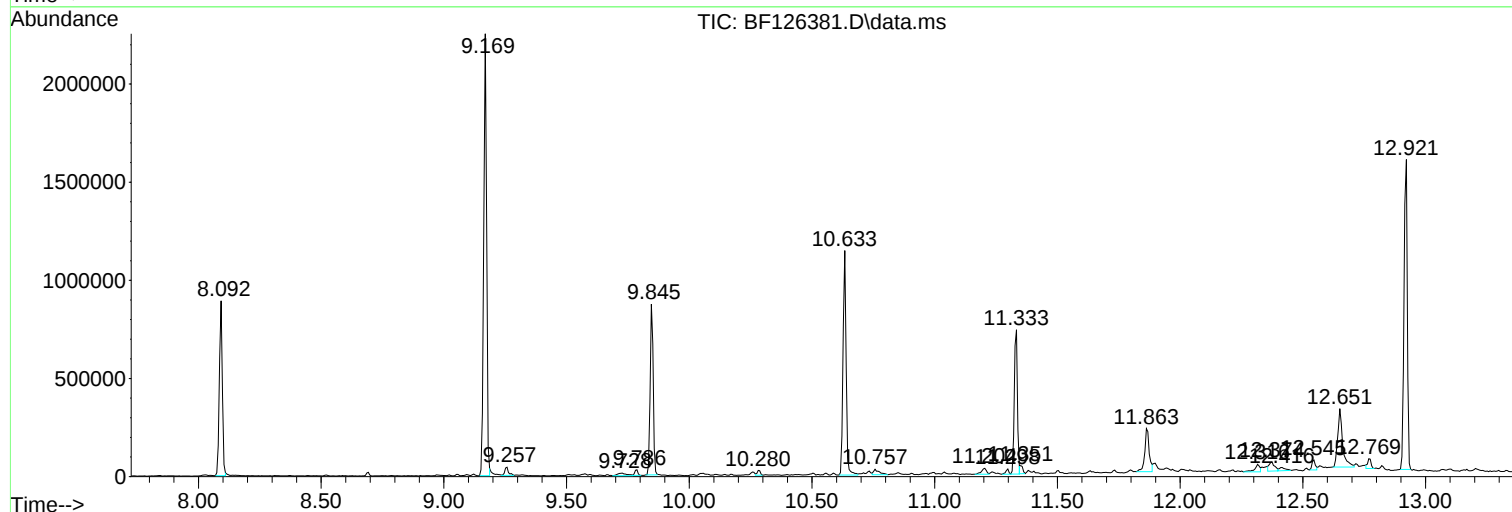
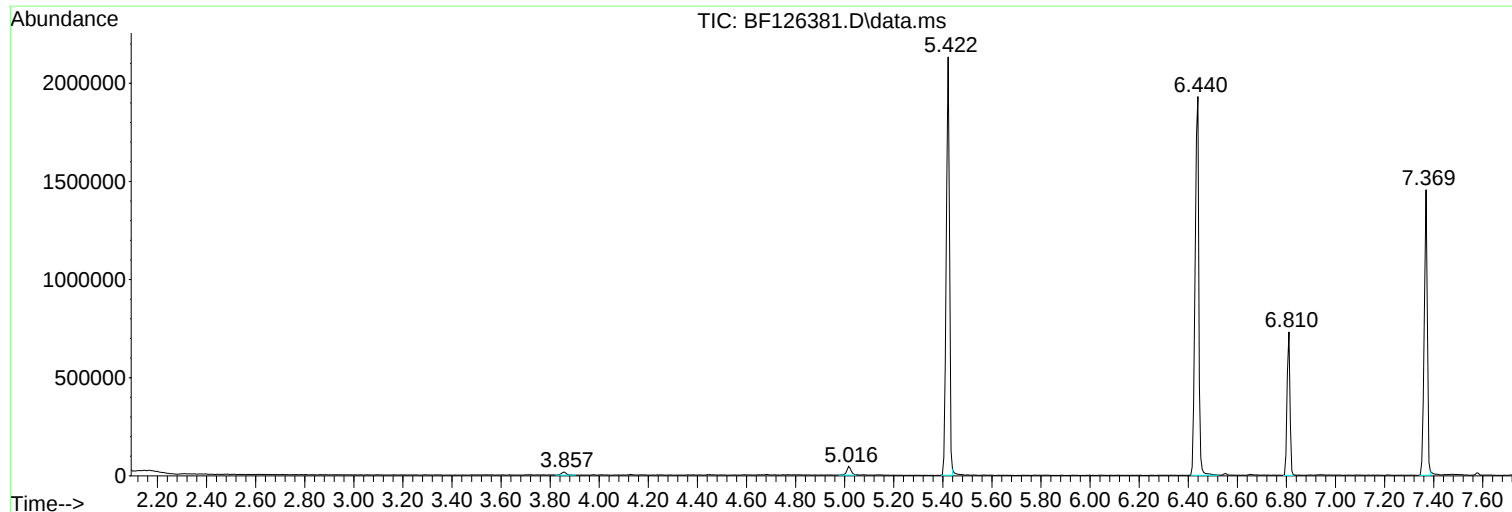
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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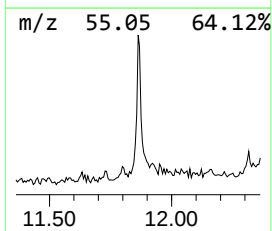
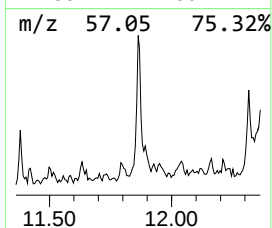
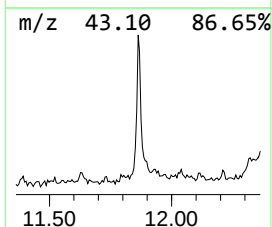
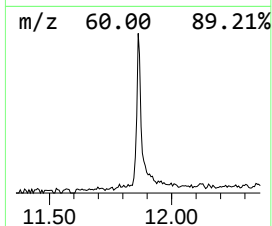
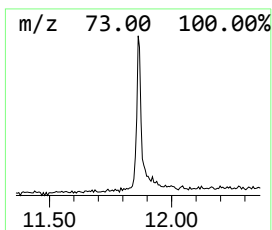
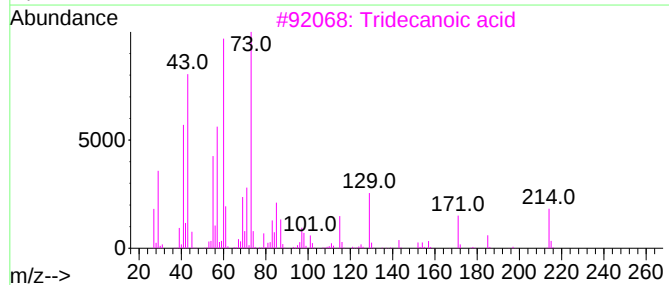
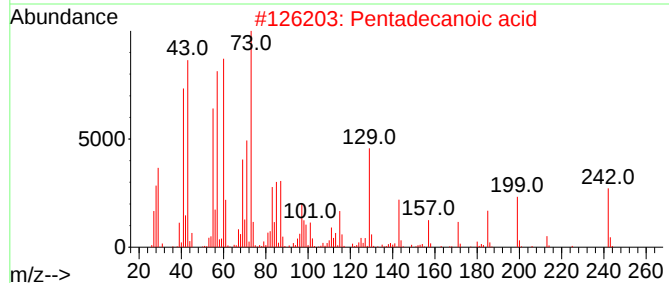
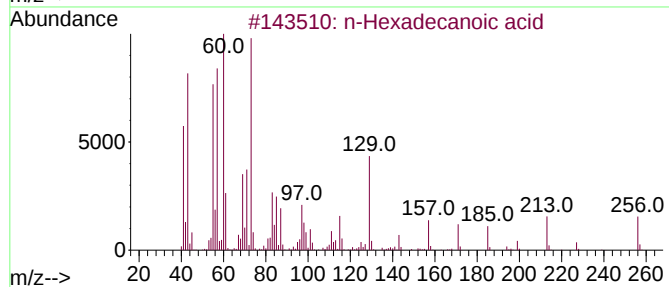
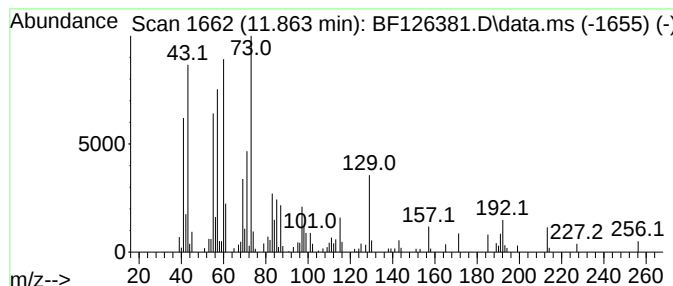
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	8.49 ng	278601	Phenanthrene-d10	11.333

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	76
4		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18
5		Dodecane	170	C12H26	000112-40-3	11



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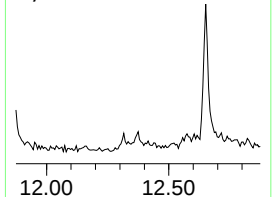
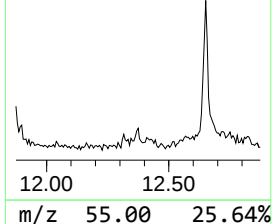
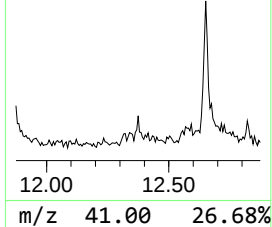
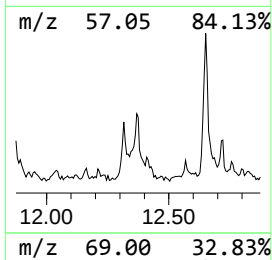
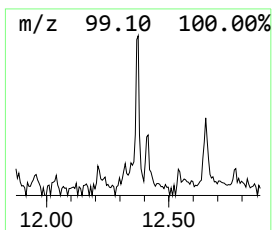
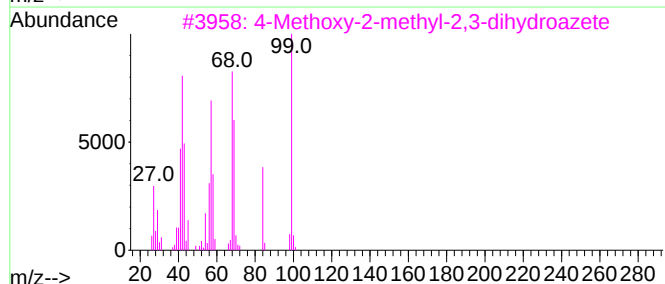
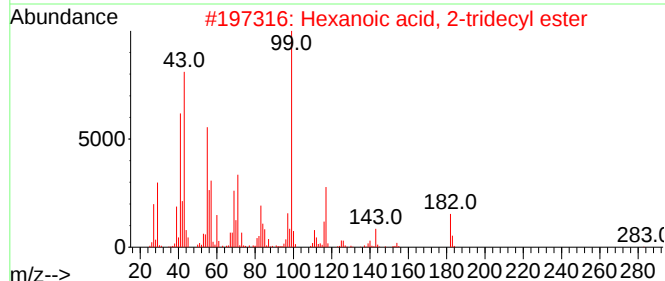
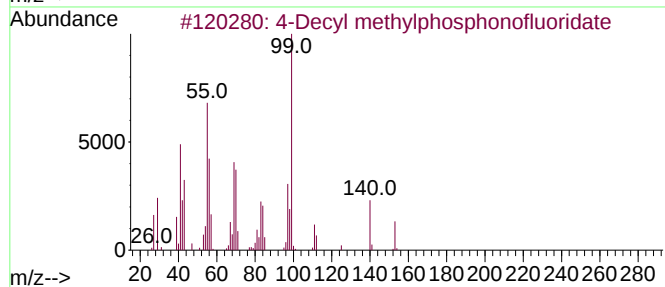
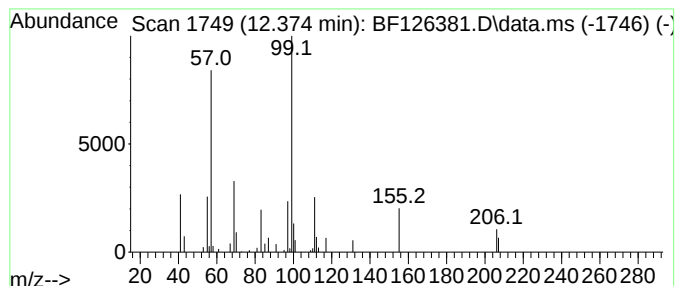
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.374 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.16 ng	71062	Phenanthrene-d10	11.333

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Decyl methylphosphonofluoridate	238	C11H24F02P	1000216-71-5	47	
2	Hexanoic acid, 2-tridecyl ester	298	C19H38O2	055193-20-9	33	
3	4-Methoxy-2-methyl-2,3-dihydroazete	99	C5H9NO	1000194-07-0	32	
4	1,4-Dioxaspiro[4.5]decane-6-carb...	186	C9H14O4	004746-93-4	28	
5	3,5,5-Trimethyl-1-hexyl methylph...	224	C10H22F02P	1000298-44-9	28	



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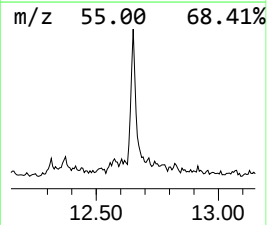
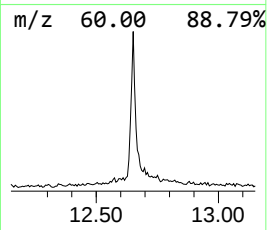
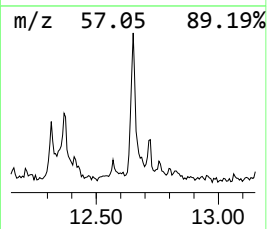
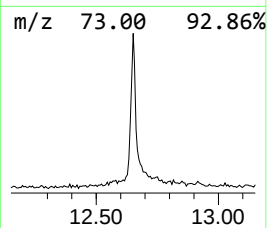
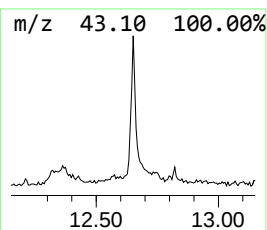
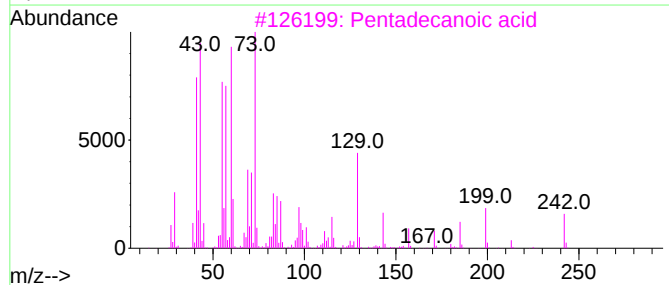
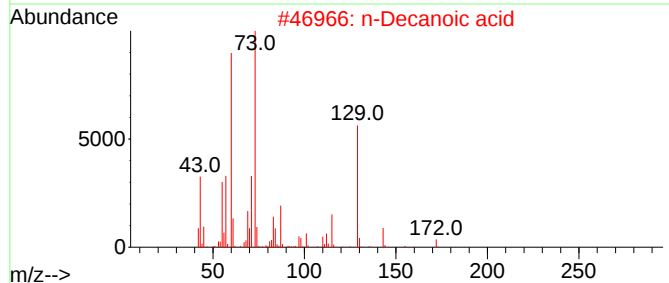
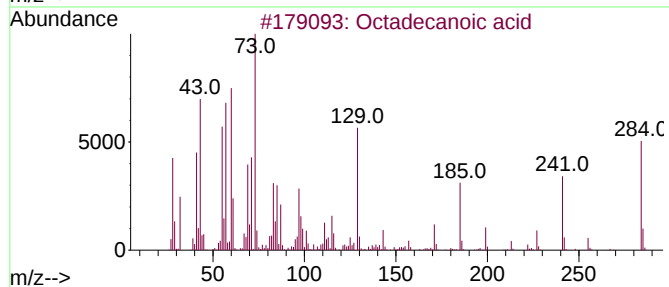
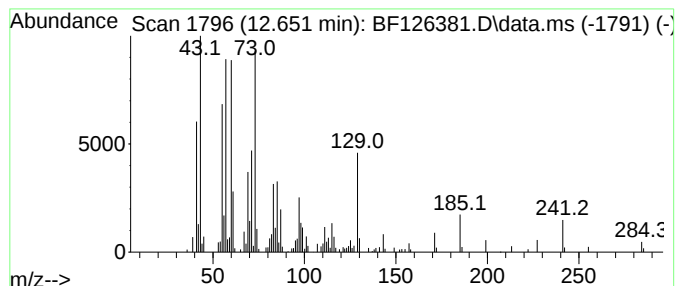
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	12.77 ng	413065	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



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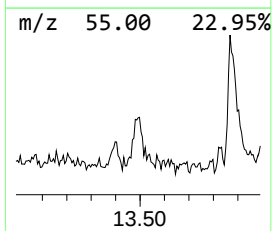
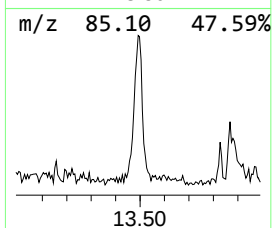
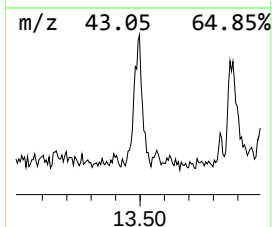
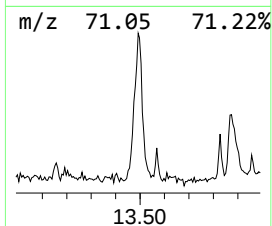
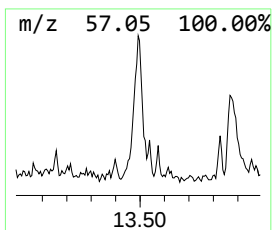
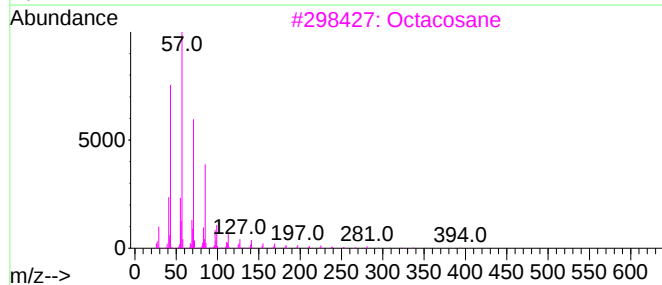
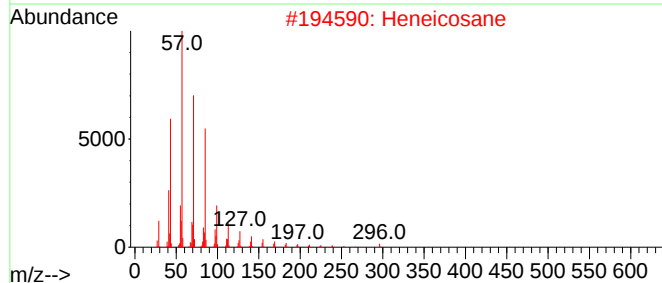
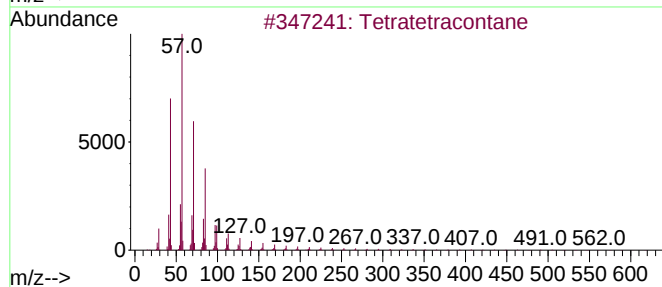
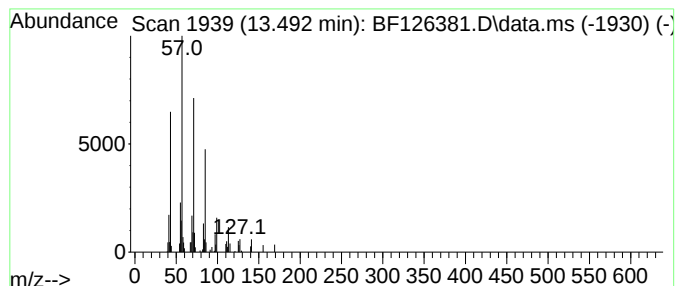
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	5.07 ng	163954	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane	296	C21H44	000629-94-7	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5			Triacosane	422	C30H62	000638-68-6	86



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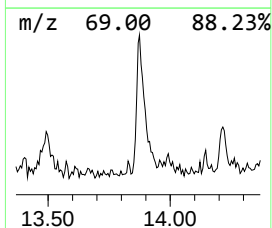
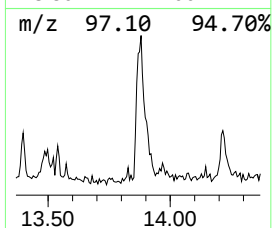
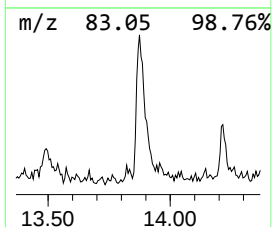
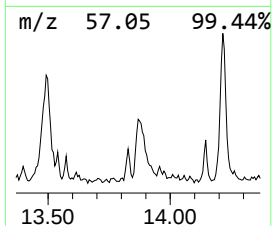
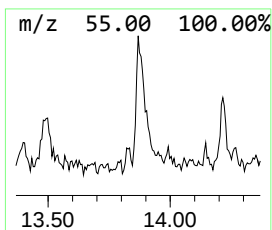
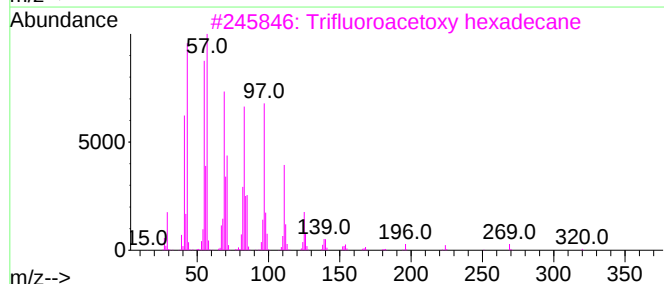
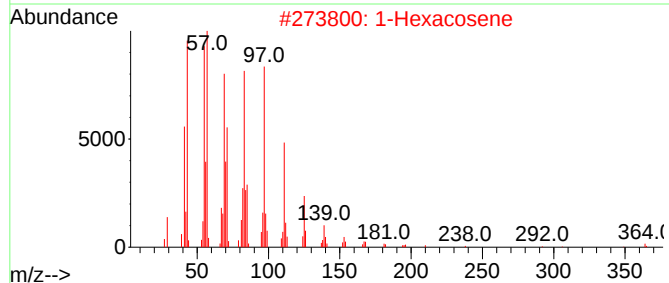
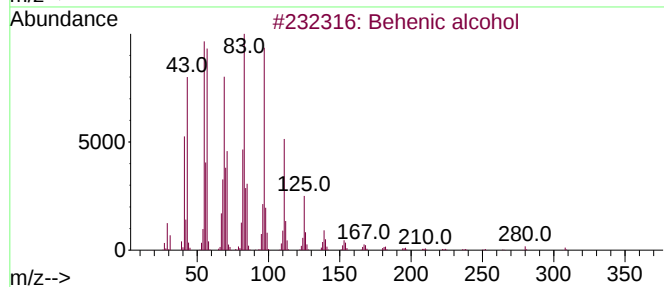
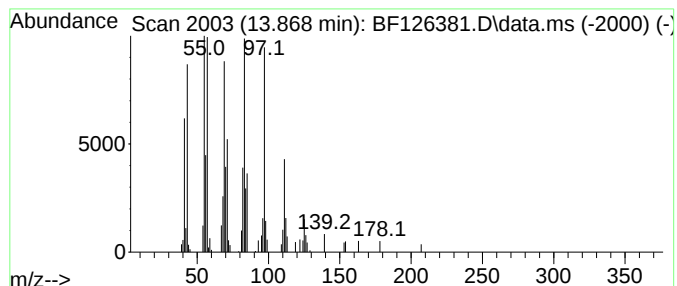
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	7.34 ng	237384	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Tricosene	322	C23H46	018835-32-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
Acq On : 28 Dec 2021 15:01
Operator : JU/CG
Sample : M5187-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-119-1-0-5

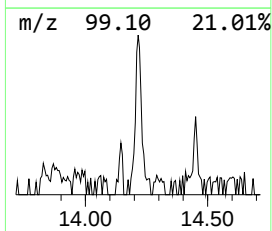
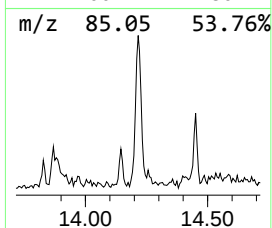
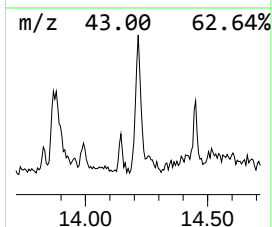
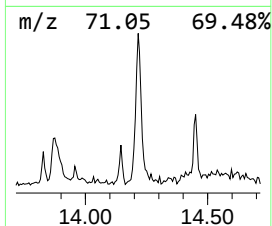
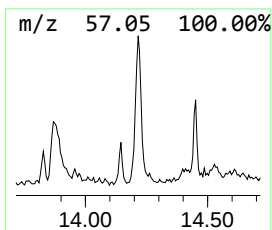
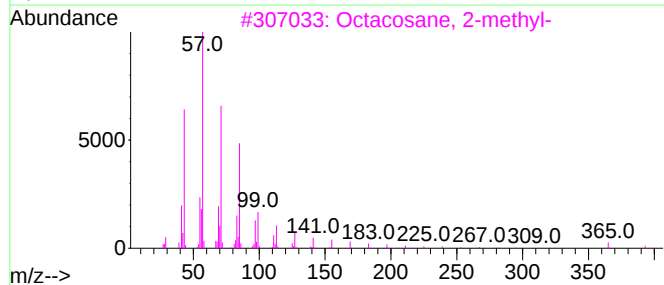
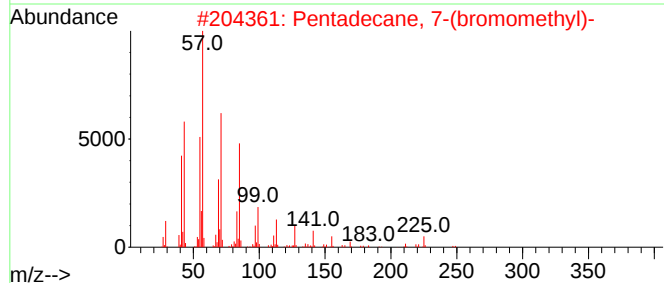
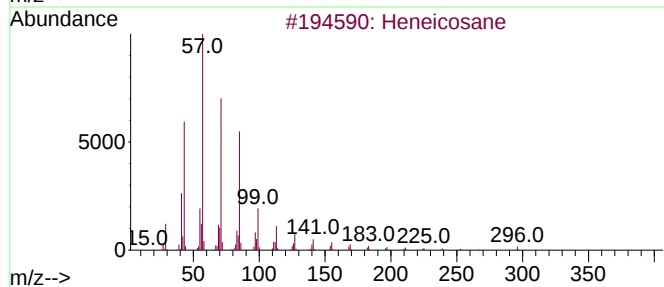
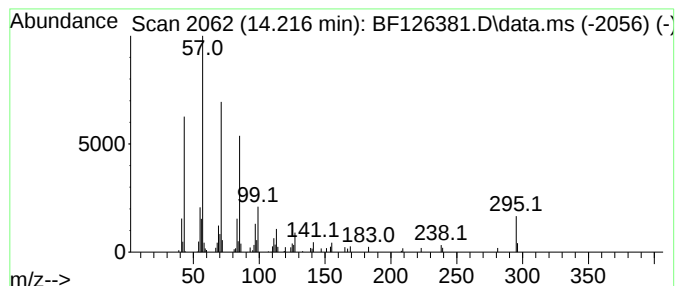
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	5.69 ng	184029	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	80
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	74
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	72
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
Acq On : 28 Dec 2021 15:01
Operator : JU/CG
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ClientSampleId :
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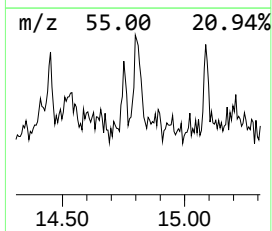
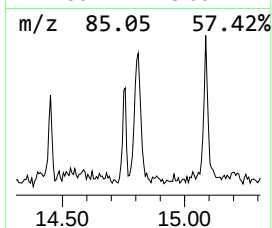
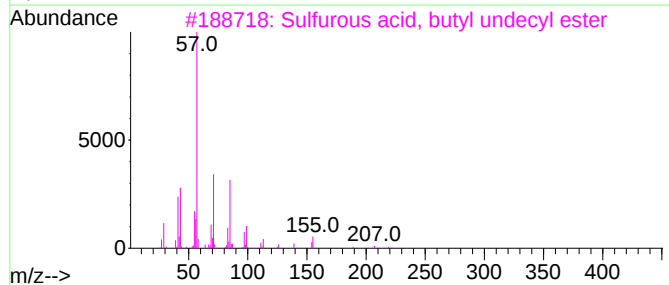
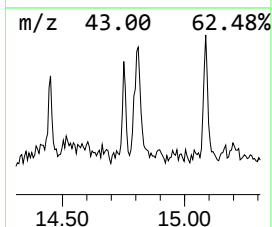
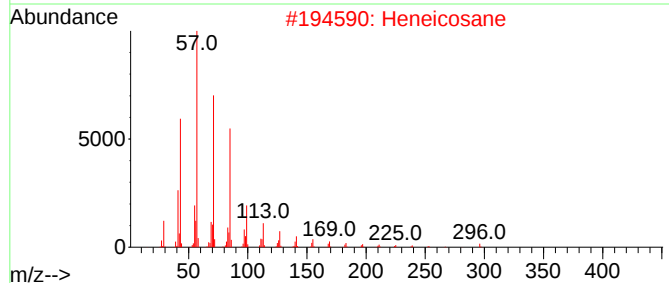
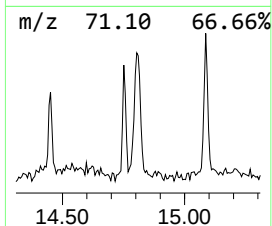
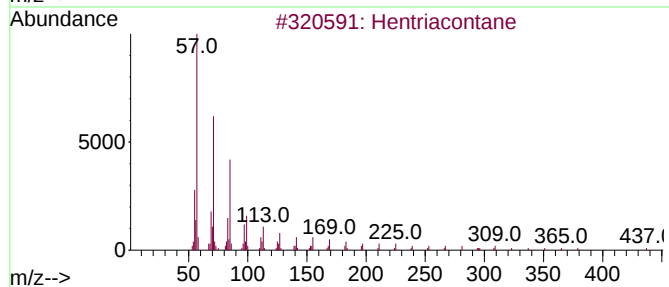
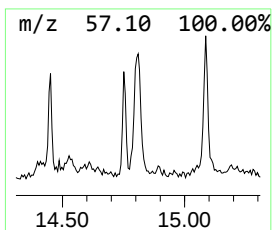
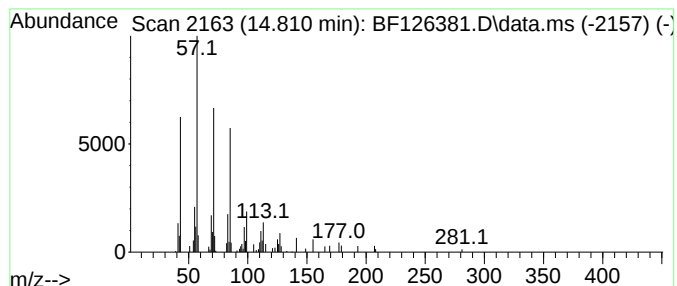
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	4.94 ng	146347	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	87
2			Heneicosane	296	C21H44	000629-94-7	87
3			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
Acq On : 28 Dec 2021 15:01
Operator : JU/CG
Sample : M5187-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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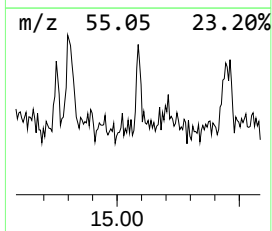
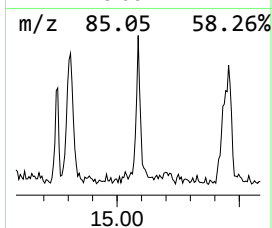
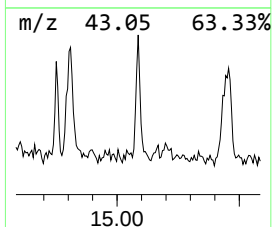
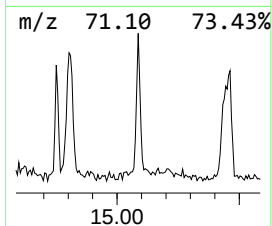
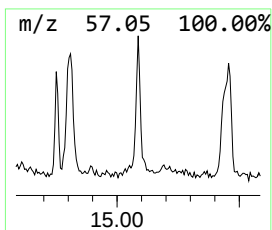
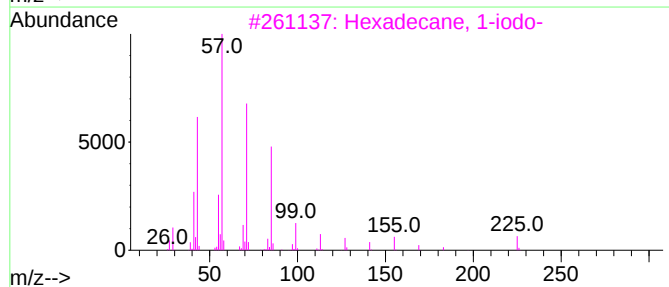
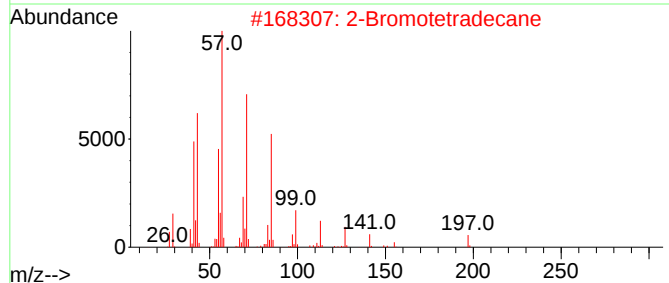
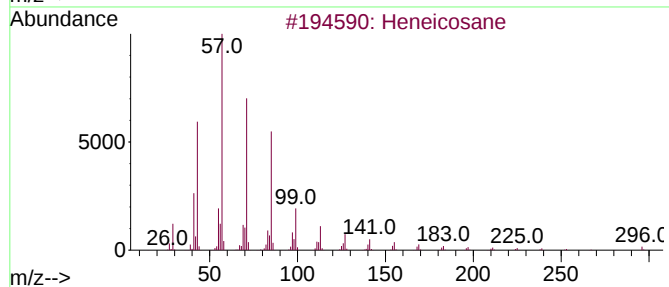
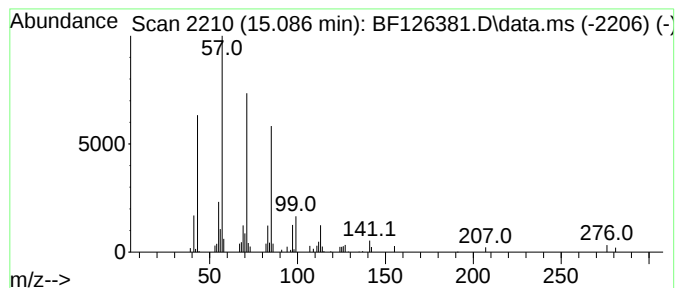
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Bromotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	2.91 ng	86309	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			2-Bromotetradecane	276	C14H29Br	074036-95-6	86
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	78
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	78
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
Acq On : 28 Dec 2021 15:01
Operator : JU/CG
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Instrument :
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ClientSampleId :
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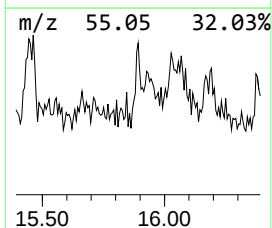
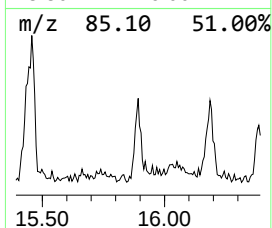
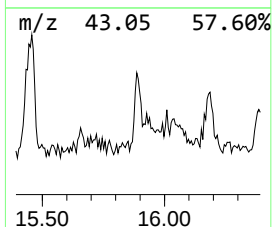
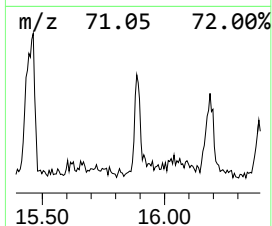
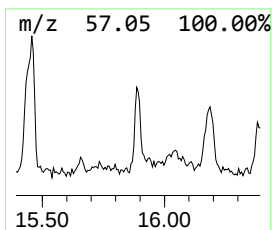
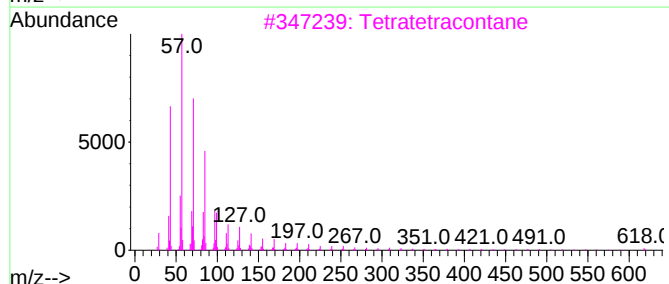
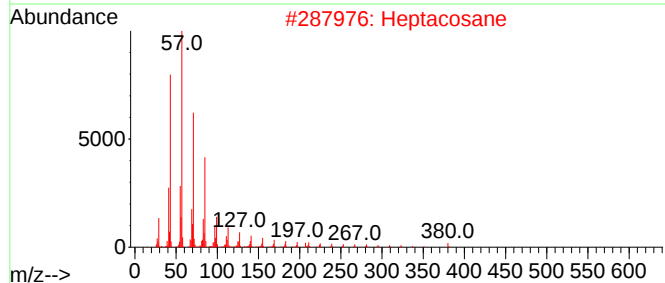
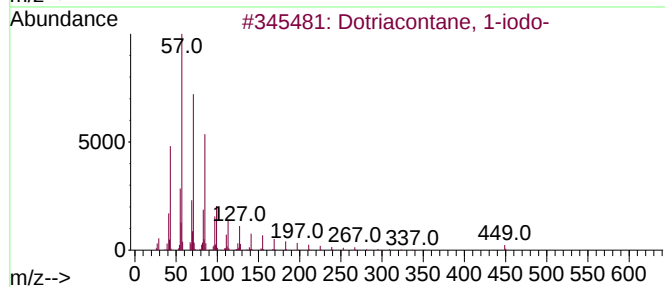
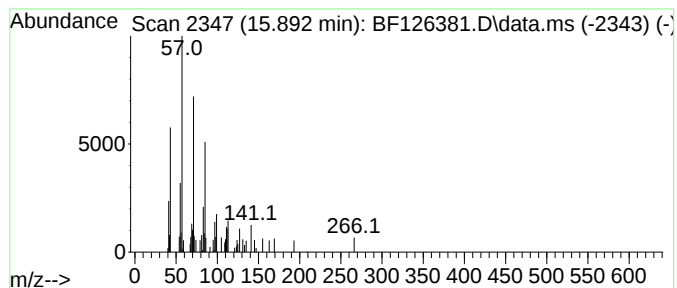
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dotriacontane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.02 ng	59742	Perylene-d12	15.421

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
2		Heptacosane	380	C27H56	000593-49-7	86
3		Tetratetracontane	619	C44H90	007098-22-8	86
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
5		Pentacosane	352	C25H52	000629-99-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
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Sample : M5187-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

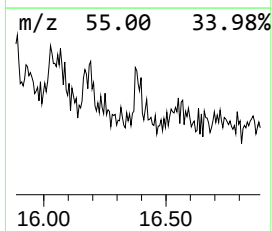
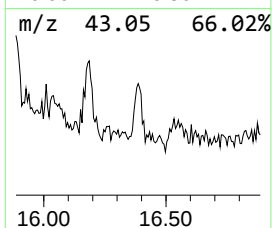
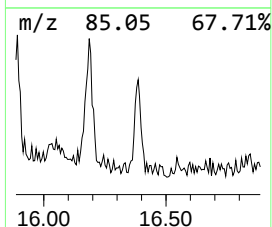
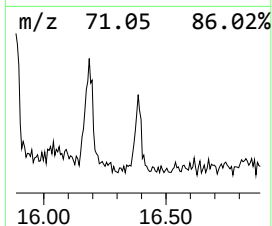
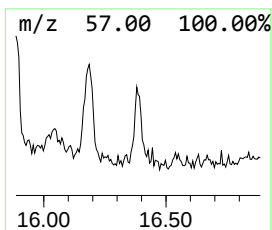
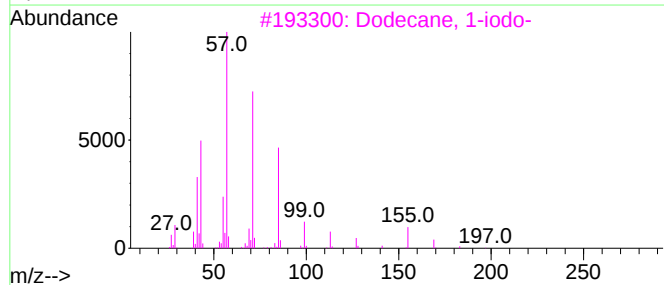
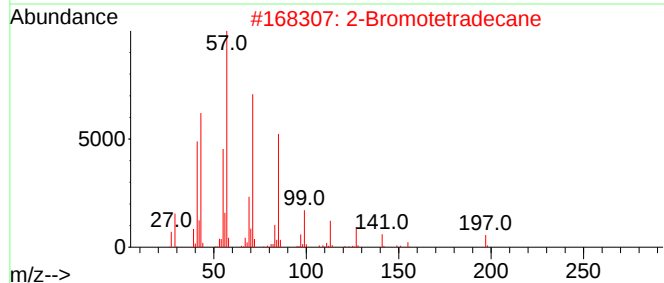
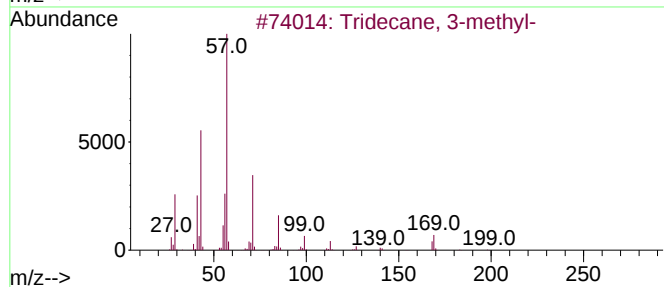
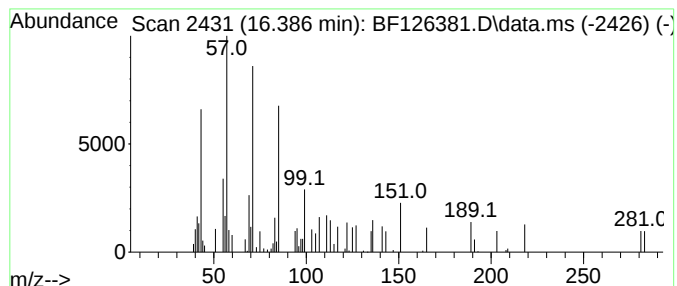
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.386 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.386	2.43 ng	71880	Perylene-d12		15.421	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-		198	C14H30	006418-41-3	47
2	2-Bromotetradecane		276	C14H29Br	074036-95-6	47
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	47
4	Hentriacontane		437	C31H64	000630-04-6	47
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
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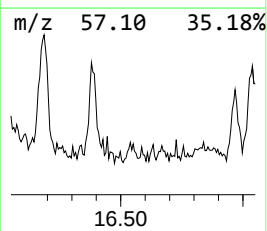
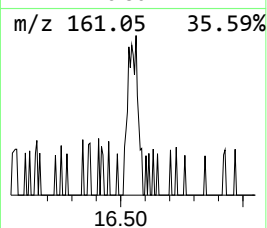
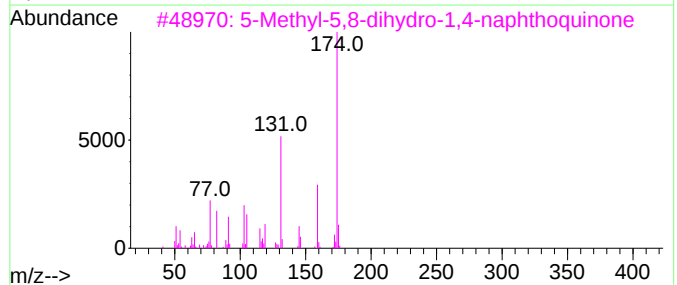
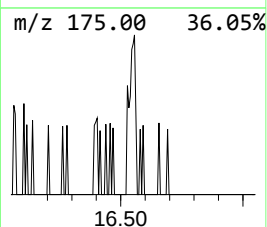
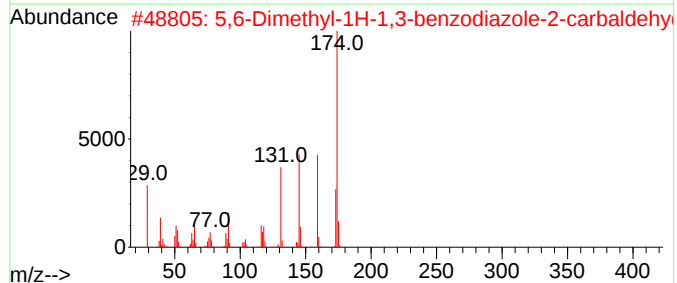
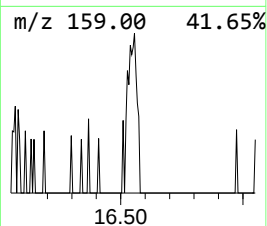
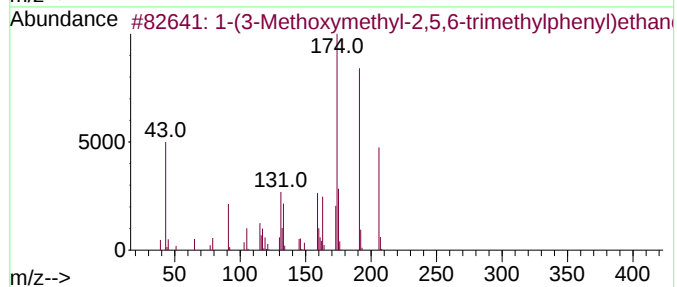
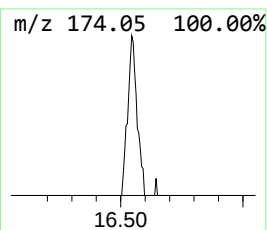
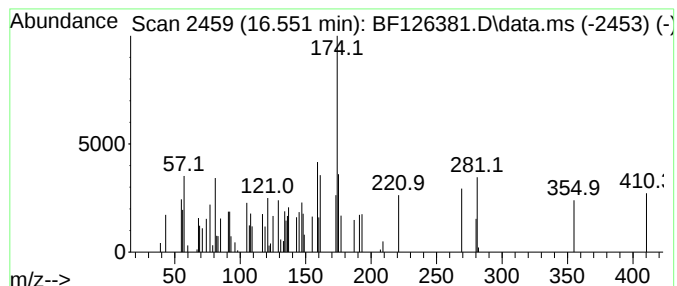
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.551 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	2.15 ng	63725	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Methoxymethyl-2,5,6-trimeth...	206	C13H18O2	1000202-04-3	38		
2	5,6-Dimethyl-1H-1,3-benzodiazole...	174	C10H10N2O	920484-85-1	37		
3	5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	35		
4	(1S,2R)-1,2,3,4-Tetrahydro-5-met...	275	C17H25NO2	1000498-70-2	32		
5	3-(3-Methoxyphenyl)-1H-pyrazole	174	C10H10N2O	1000410-63-5	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126381.D
Acq On : 28 Dec 2021 15:01
Operator : JU/CG
Sample : M5187-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.863	8.5	ng	278601	4	11.333	656528	20.0
unknown12.374	12.374	2.2	ng	71062	4	11.333	656528	20.0
Octadecanoic acid	12.651	12.8	ng	413065	5	13.969	646916	20.0
Tetratetracontane	13.492	5.1	ng	163954	5	13.969	646916	20.0
2,2'-(Ethane-1,...	13.845	2.3	ng	75743	5	13.969	646916	20.0
Behenic alcohol	13.868	7.3	ng	237384	5	13.969	646916	20.0
Heneicosane	14.216	5.7	ng	184029	5	13.969	646916	20.0
Hentriacontane	14.810	4.9	ng	146347	6	15.421	592368	20.0
2-Bromotetradecane	15.086	2.9	ng	86309	6	15.421	592368	20.0
Dotriacontane, ...	15.892	2.0	ng	59742	6	15.421	592368	20.0
unknown16.386	16.386	2.4	ng	71880	6	15.421	592368	20.0
unknown16.551	16.551	2.1	ng	63725	6	15.421	592368	20.0