

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
 Data File : BF125595.D
 Acq On : 23 Sep 2021 16:54
 Operator : JU/CG
 Sample : M3824-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-C

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-BF092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	12	21	26	rBV	1251456	1588768	25.89%	3.615%
2	5.516	577	583	586	rBV	4849777	4737767	77.22%	10.781%
3	6.516	747	753	756	rBV	4325493	4685504	76.37%	10.662%
4	6.892	814	817	821	rBV	1300379	1050405	17.12%	2.390%
5	7.451	907	912	915	rBV	3202946	3094986	50.44%	7.043%
6	8.075	1014	1018	1026	rBV	268674	251623	4.10%	0.573%
7	8.175	1031	1035	1038	rBV	1840718	1466341	23.90%	3.337%
8	9.251	1213	1218	1221	rBV	6209289	5936944	96.76%	13.510%
9	9.927	1329	1333	1337	rBV	1811705	1683256	27.43%	3.830%
10	10.716	1462	1467	1471	rBV	3668429	3812674	62.14%	8.676%
11	11.416	1582	1586	1589	rBV	2151511	1730877	28.21%	3.939%
12	11.945	1669	1676	1695	rBV	1255141	1646575	26.84%	3.747%
13	12.221	1712	1723	1735	rVB5	73183	271387	4.42%	0.618%
14	12.627	1786	1792	1794	rBV3	55132	66199	1.08%	0.151%
15	12.727	1804	1809	1815	rBV	844496	892583	14.55%	2.031%
16	13.004	1851	1856	1859	rBV	6031914	6135434	100.00%	13.962%
17	13.604	1955	1958	1964	rVB	79355	111341	1.81%	0.253%
18	13.898	2003	2008	2018	rBV3	354908	512112	8.35%	1.165%
19	14.057	2030	2035	2038	rBV	1727464	1626014	26.50%	3.700%
20	14.227	2058	2064	2071	rBV	123502	188302	3.07%	0.429%
21	14.527	2112	2115	2127	rVB2	71166	100826	1.64%	0.229%
22	14.757	2147	2154	2158	rBV	76249	122822	2.00%	0.279%
23	14.839	2160	2168	2173	rVV3	82564	181599	2.96%	0.413%
24	15.186	2223	2227	2232	rBV	59780	69834	1.14%	0.159%
25	15.327	2246	2251	2262	rVB	57571	110017	1.79%	0.250%
26	15.533	2281	2286	2291	rBV	1181627	1472863	24.01%	3.352%
27	15.574	2291	2293	2301	rVB	63037	85244	1.39%	0.194%
28	16.080	2374	2379	2387	rBV4	34399	75021	1.22%	0.171%
29	16.745	2485	2492	2499	rVB8	24807	67385	1.10%	0.153%
30	17.156	2557	2562	2569	rBV6	36072	85132	1.39%	0.194%
31	17.645	2638	2645	2653	rBV10	29355	84574	1.38%	0.192%

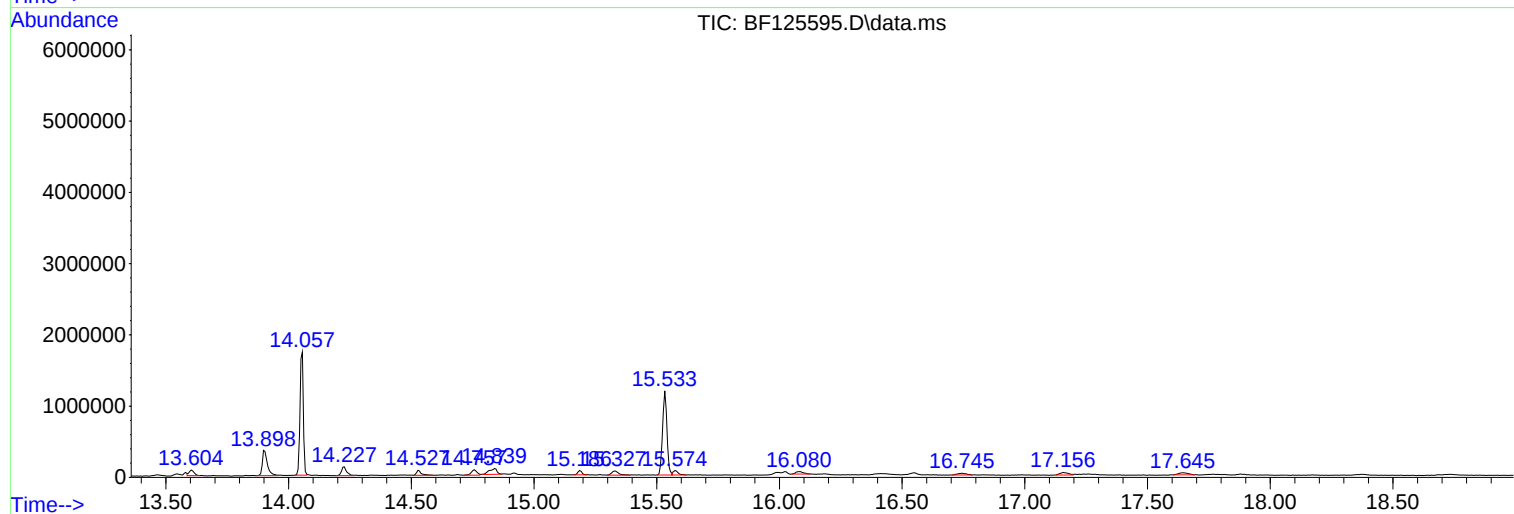
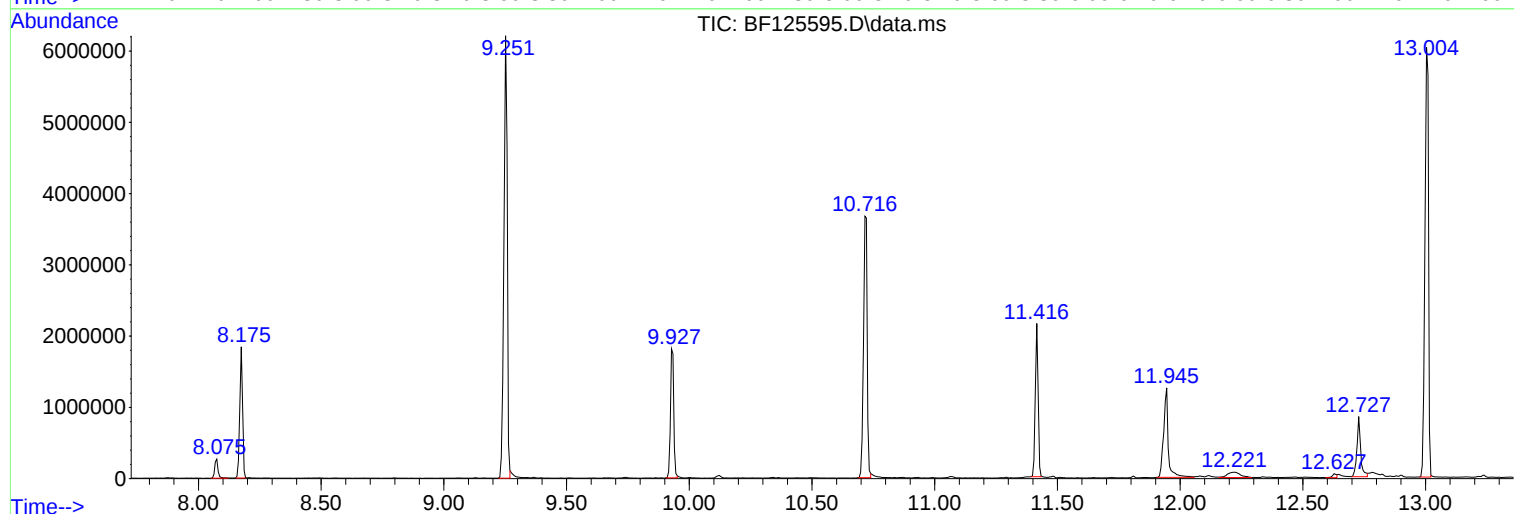
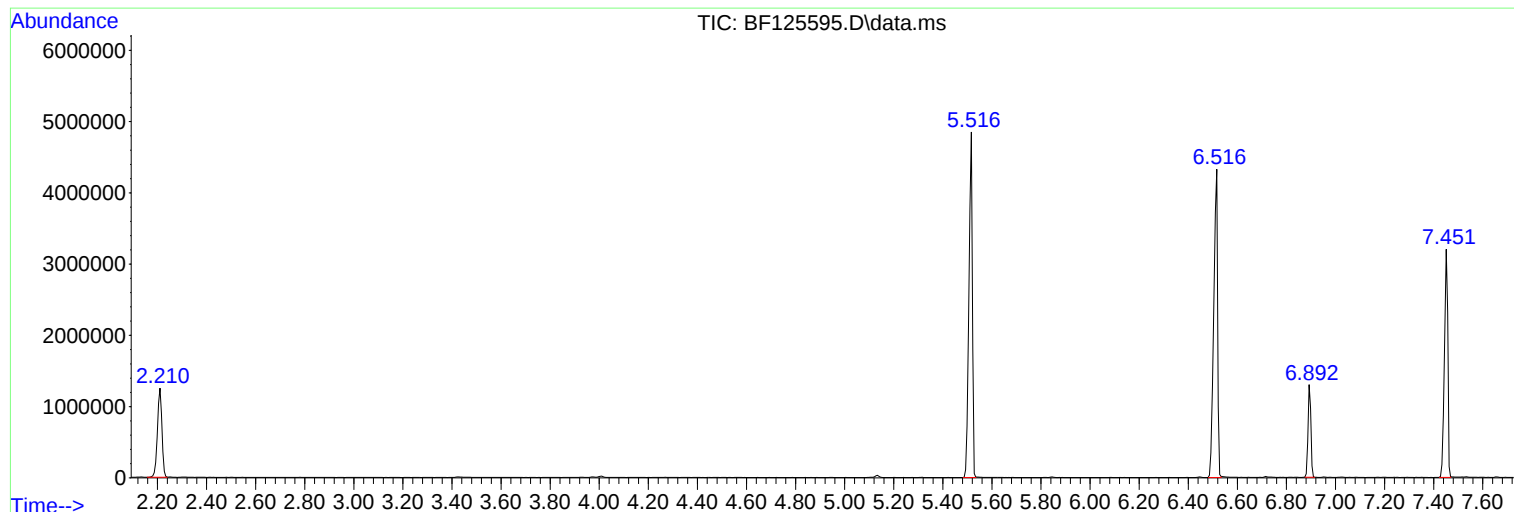
Sum of corrected areas: 43944409

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

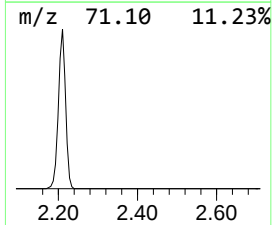
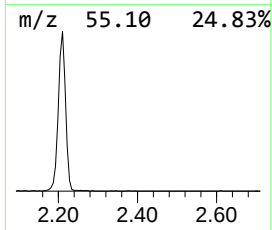
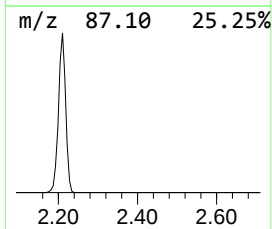
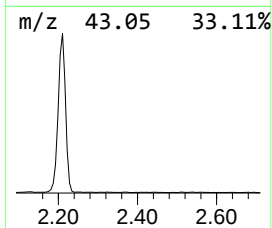
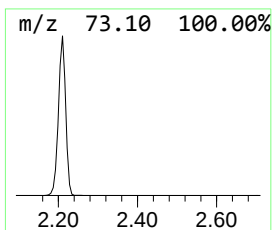
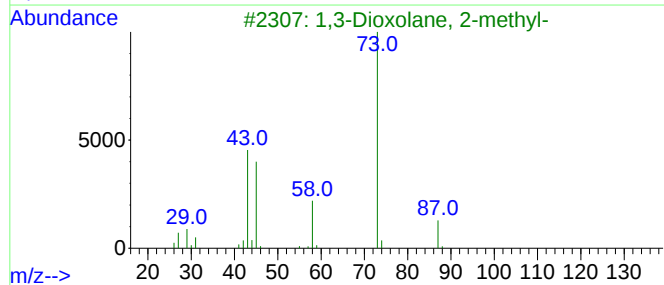
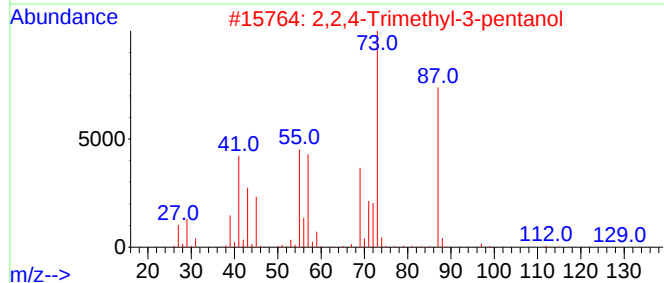
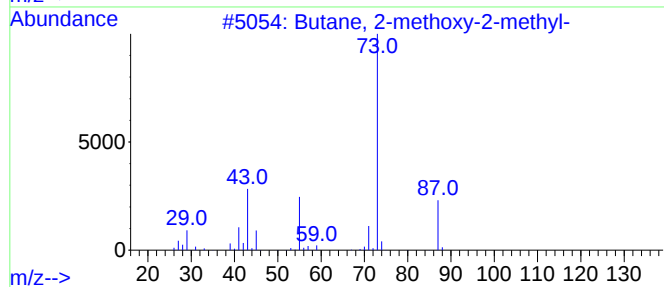
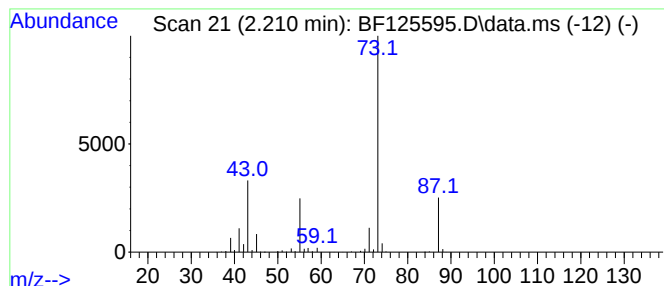
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	30.25 ng	1588770	1,4-Dichlorobenzene-d4	6.892

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

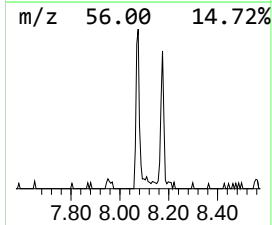
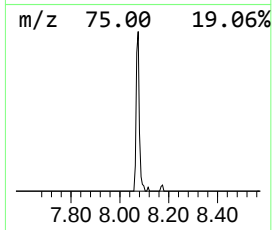
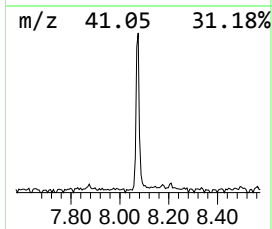
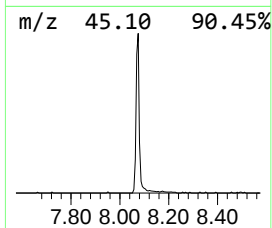
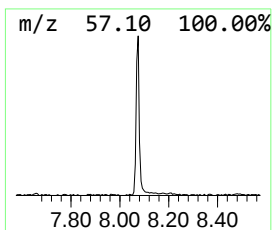
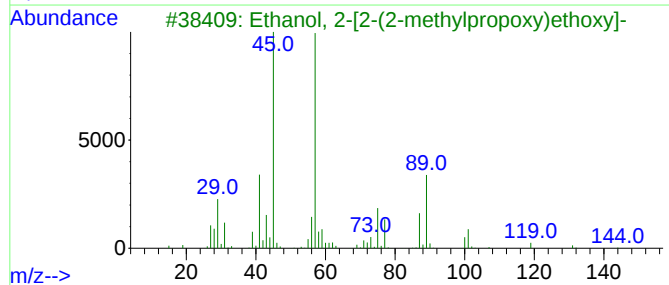
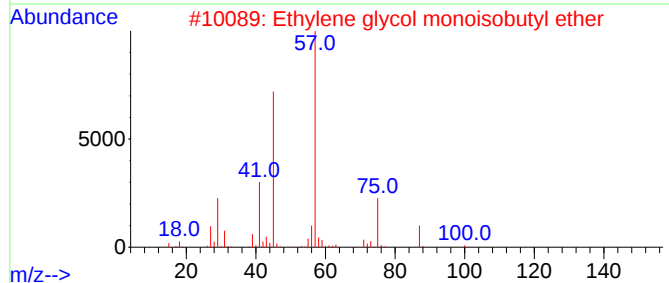
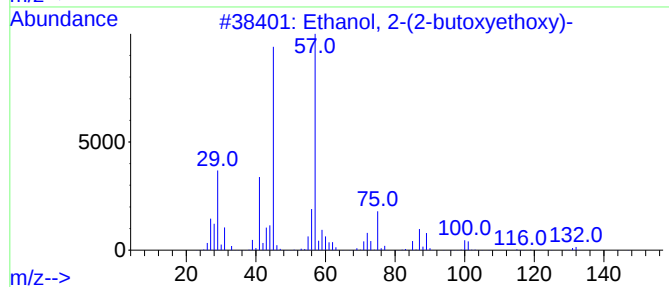
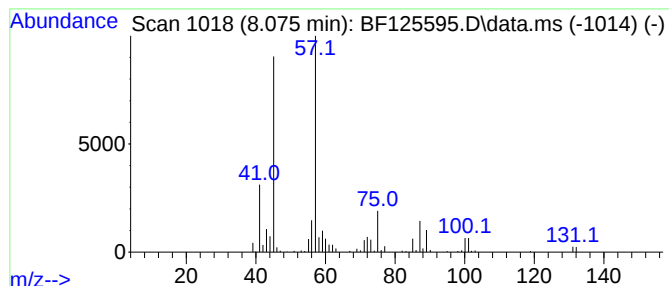
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	3.43 ng	251623	Naphthalene-d8	8.175

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			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

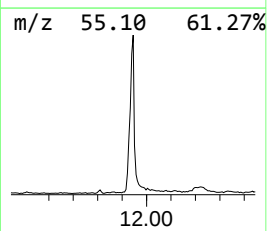
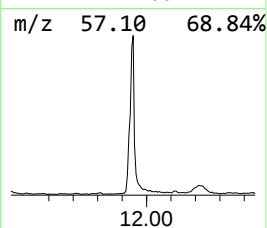
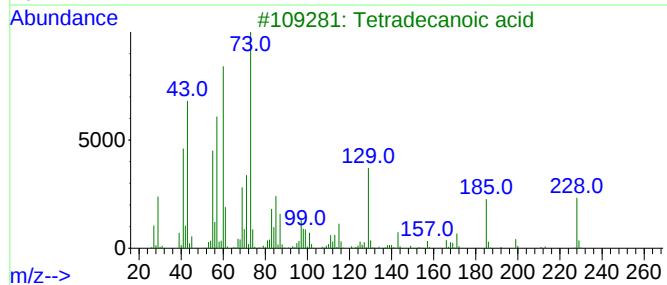
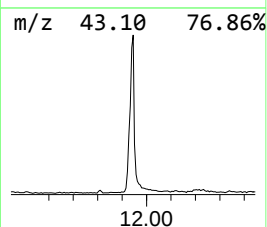
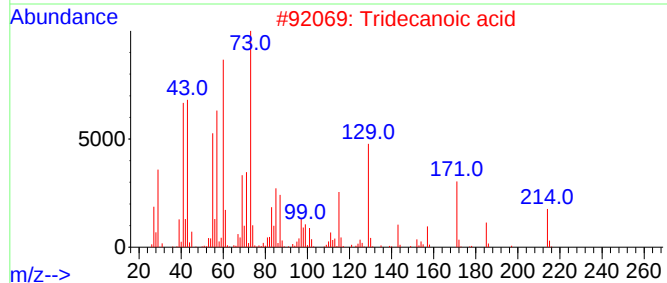
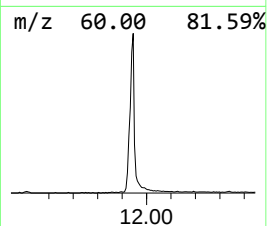
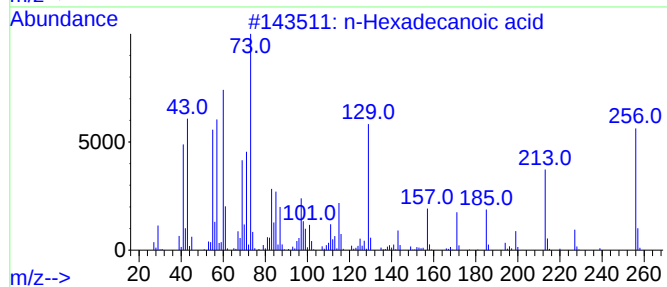
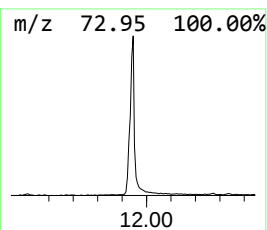
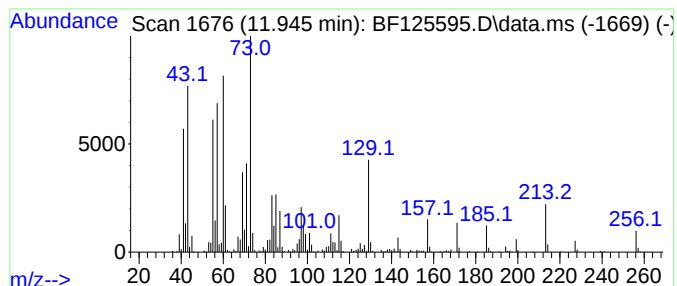
Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.945	19.03 ng	1646580	Phenanthrene-d10		11.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	n-Decanoic acid		172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

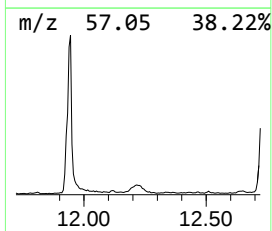
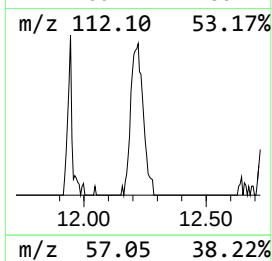
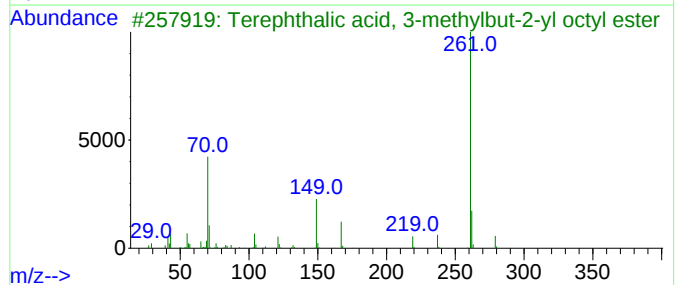
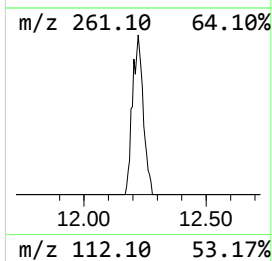
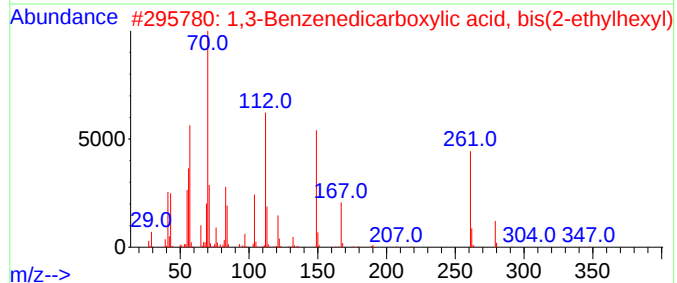
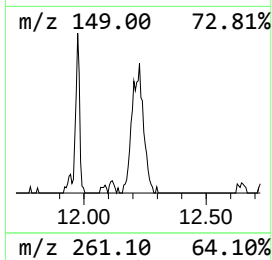
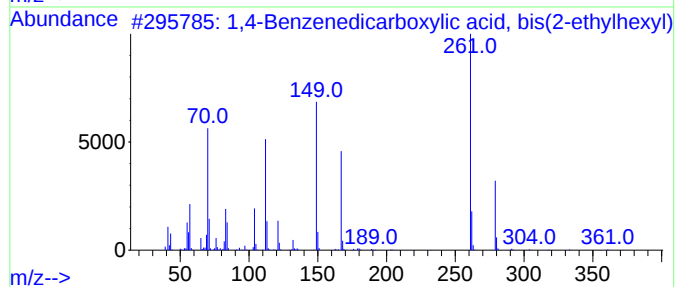
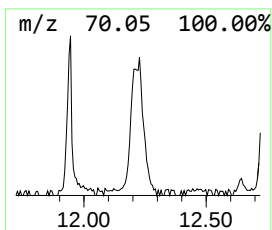
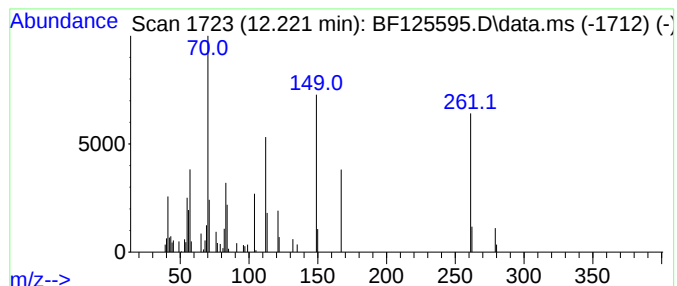
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.221	3.14 ng	271387	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	91
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	81
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
4			Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	35
5			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

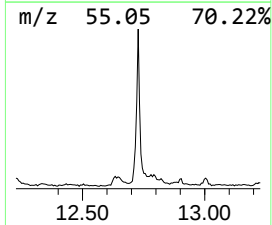
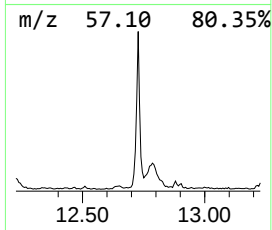
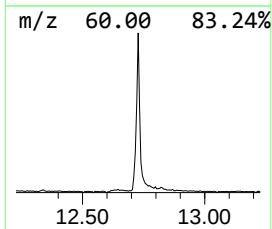
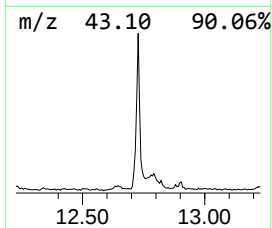
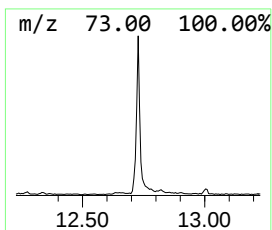
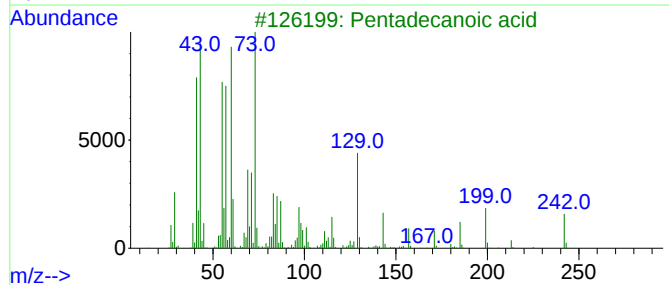
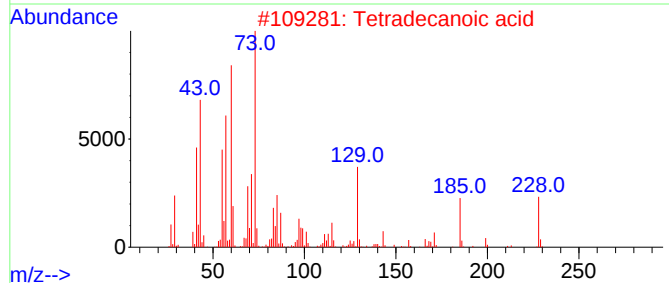
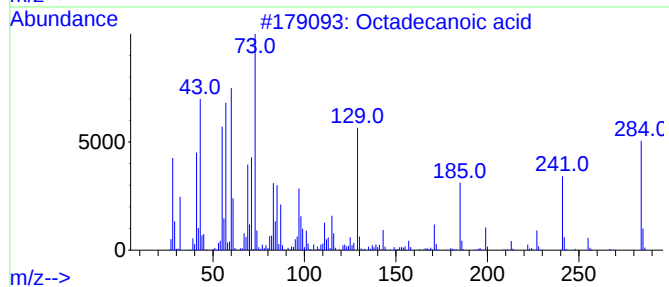
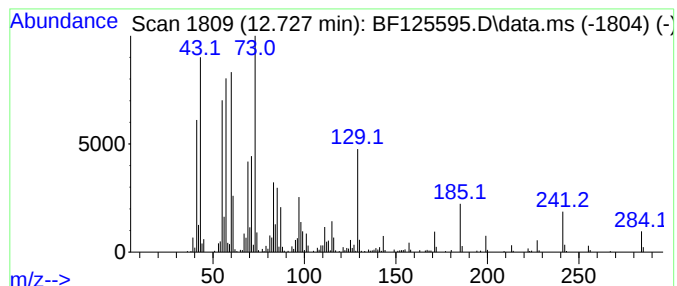
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	10.31 ng	892583	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

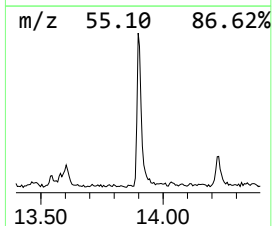
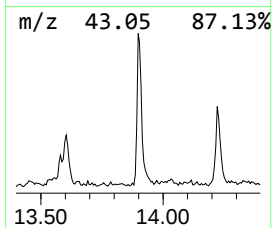
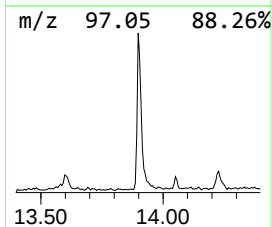
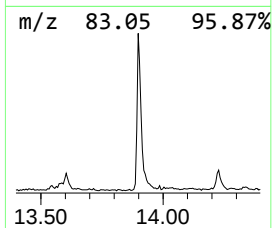
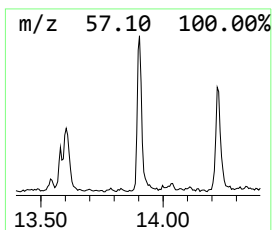
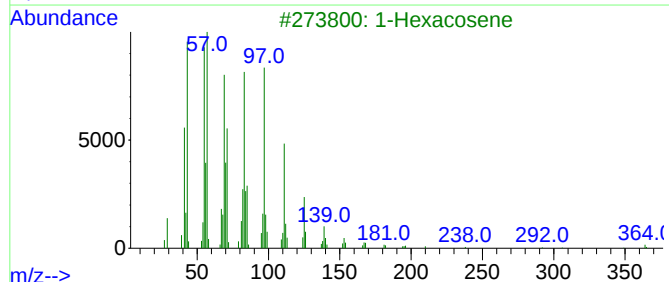
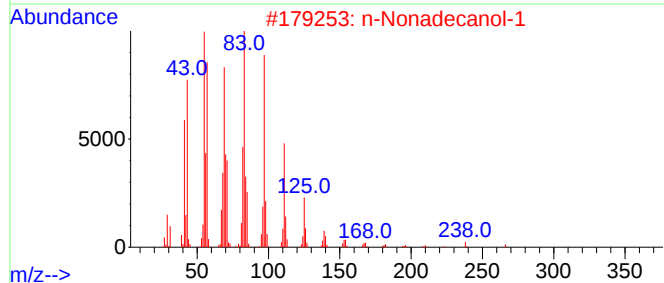
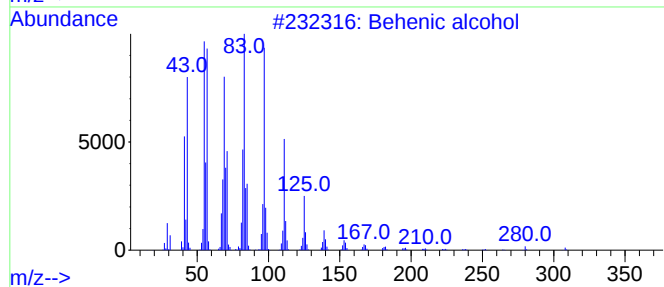
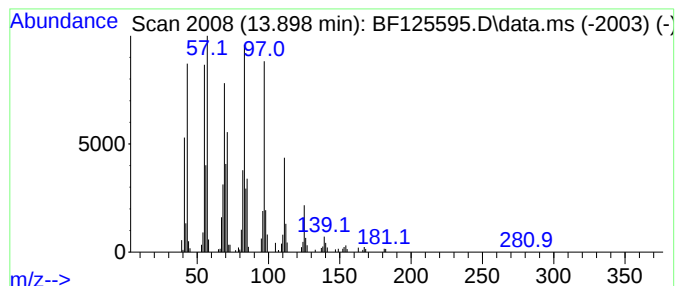
Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
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 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.898	6.30 ng	512112	Chrysene-d12		14.057	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Behenic alcohol		326	C22H46O	000661-19-8	95
2	n-Nonadecanol-1		284	C19H40O	001454-84-8	95
3	1-Hexacosene		364	C26H52	018835-33-1	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	93
5	3-Eicosene, (E)-		280	C20H40	074685-33-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

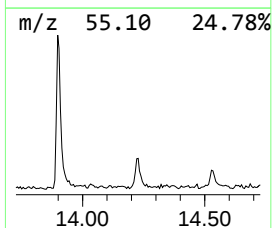
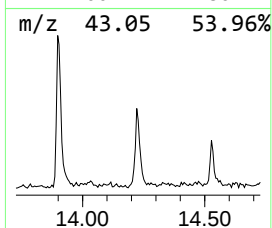
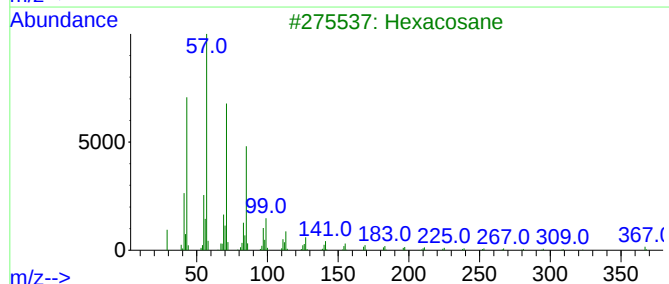
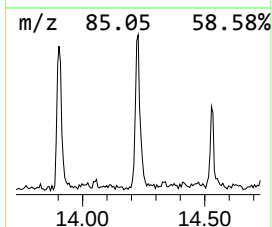
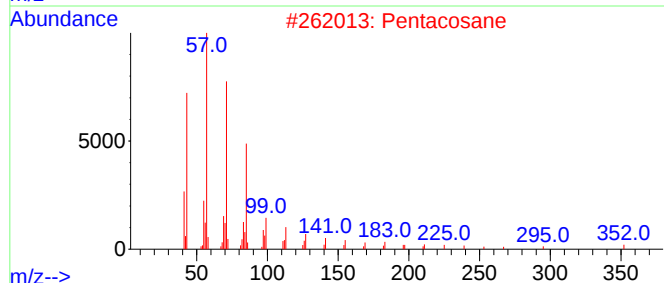
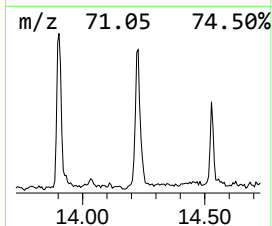
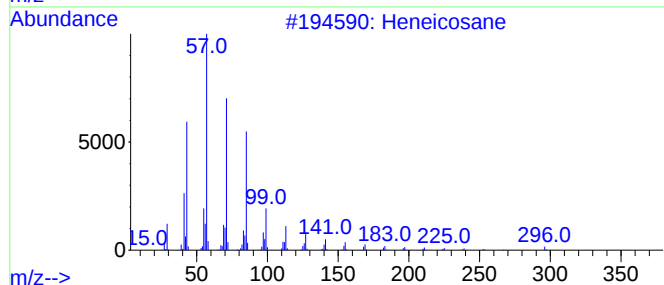
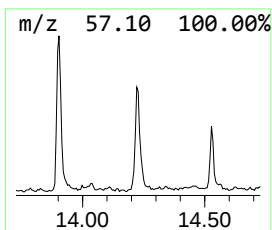
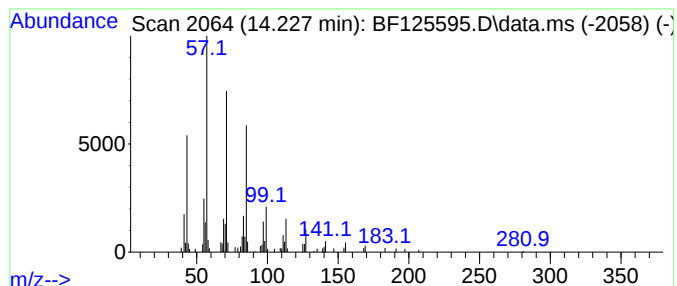
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	2.32 ng	188302	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

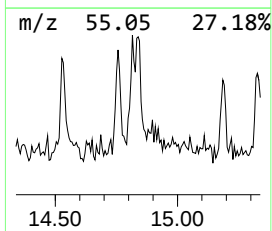
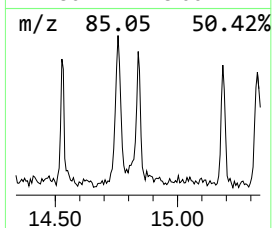
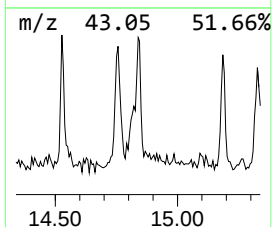
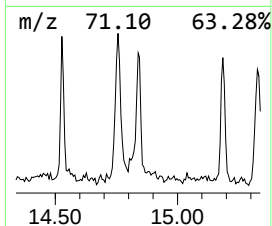
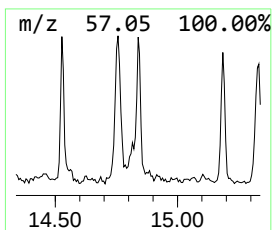
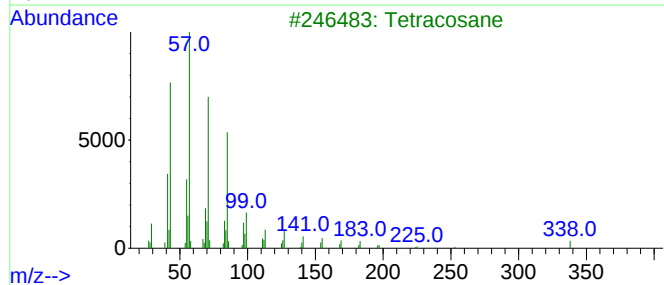
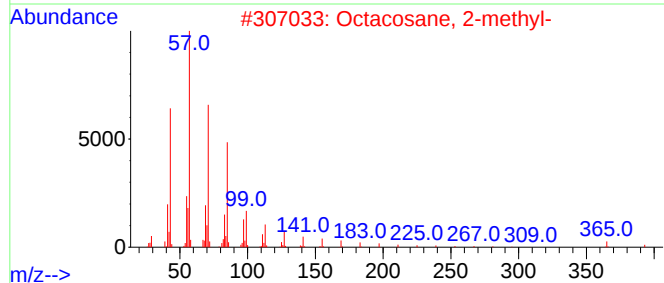
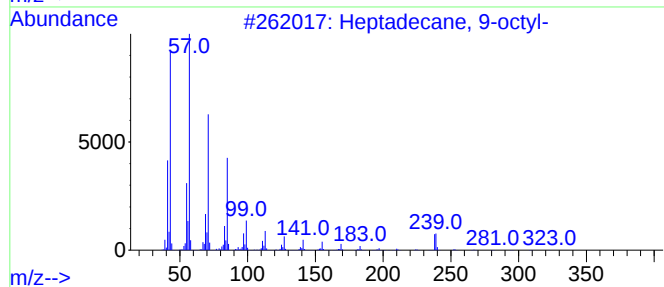
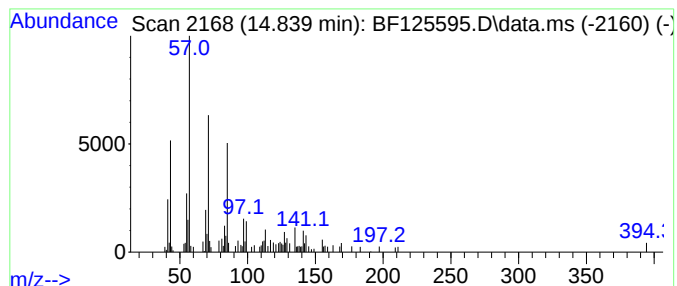
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.47 ng	181599	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Tetracosane	338	C24H50	000646-31-1	87
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125595.D
Acq On : 23 Sep 2021 16:54
Operator : JU/CG
Sample : M3824-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.210	30.3	ng	1588770	1	6.892	1050410	20.0
Ethanol, 2-(2-b...	8.075	3.4	ng	251623	2	8.175	1466340	20.0
n-Hexadecanoic ...	11.945	19.0	ng	1646580	4	11.416	1730880	20.0
1,4-Benzenedica...	12.221	3.1	ng	271387	4	11.416	1730880	20.0
Octadecanoic acid	12.727	10.3	ng	892583	4	11.416	1730880	20.0
Behenic alcohol	13.898	6.3	ng	512112	5	14.057	1626010	20.0
Heneicosane	14.227	2.3	ng	188302	5	14.057	1626010	20.0
Heptadecane, 9-...	14.839	2.5	ng	181599	6	15.533	1472860	20.0