

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
 Data File : BF126079.D
 Acq On : 9 Nov 2021 13:13
 Operator : JU/CG
 Sample : M4540-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126079.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	13	19	rBV	1963021	2485441	47.07%	6.424%
2	5.081	506	509	515	rVB	53661	63273	1.20%	0.164%
3	5.475	570	576	579	rBV	4790388	4454224	84.36%	11.512%
4	6.481	741	747	750	rBV	4623023	4631337	87.72%	11.970%
5	6.851	806	810	813	rBV	1310867	986215	18.68%	2.549%
6	7.410	900	905	908	rBV	3034449	3066664	58.08%	7.926%
7	8.034	1007	1011	1022	rBV	648921	690177	13.07%	1.784%
8	8.134	1024	1028	1031	rBV	1471438	1251261	23.70%	3.234%
9	9.210	1206	1211	1214	rBV	5935555	5279863	100.00%	13.646%
10	9.739	1298	1301	1304	rBV	113710	89930	1.70%	0.232%
11	9.863	1318	1322	1323	rBV	341223	268476	5.08%	0.694%
12	9.886	1323	1326	1329	rVB	1766171	1418733	26.87%	3.667%
13	10.675	1455	1460	1463	rBV	4122068	3577157	67.75%	9.245%
14	11.369	1574	1578	1581	rBV	1711888	1450205	27.47%	3.748%
15	11.439	1584	1590	1593	rVB5	52488	57832	1.10%	0.149%
16	11.898	1665	1668	1672	rBV	154987	132348	2.51%	0.342%
17	12.580	1782	1784	1788	rVB	79786	61136	1.16%	0.158%
18	12.780	1815	1818	1820	rBV	79716	64970	1.23%	0.168%
19	12.957	1844	1848	1851	rBV	5162207	4162296	78.83%	10.758%
20	13.186	1881	1887	1892	rVB6	32025	62013	1.17%	0.160%
21	13.486	1935	1938	1942	rBV3	57348	67180	1.27%	0.174%
22	13.716	1973	1977	1981	rBV	682295	555192	10.52%	1.435%
23	13.857	1997	2001	2008	rBV	370484	489295	9.27%	1.265%
24	14.004	2020	2026	2030	rBV	1021322	1014275	19.21%	2.621%
25	14.180	2053	2056	2061	rBV3	45784	59540	1.13%	0.154%
26	14.498	2105	2110	2116	rBV	185891	300918	5.70%	0.778%
27	14.868	2169	2173	2177	rBV	152690	149900	2.84%	0.387%
28	15.133	2214	2218	2220	rBV	74574	80727	1.53%	0.209%
29	15.162	2220	2223	2228	rVB5	55705	78709	1.49%	0.203%
30	15.474	2270	2276	2280	rBV	785357	1006827	19.07%	2.602%
31	15.510	2280	2282	2287	rVB2	48673	64211	1.22%	0.166%
32	15.951	2353	2357	2361	rVB	89317	124238	2.35%	0.321%
33	16.009	2363	2367	2374	rBV3	57182	129517	2.45%	0.335%
34	16.457	2439	2443	2451	rVB4	44621	69883	1.32%	0.181%
35	17.051	2539	2544	2551	rBV3	49649	98334	1.86%	0.254%
36	17.545	2621	2628	2642	rBV3	53802	149238	2.83%	0.386%

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Instrument :
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ClientSampleId :
TP-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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

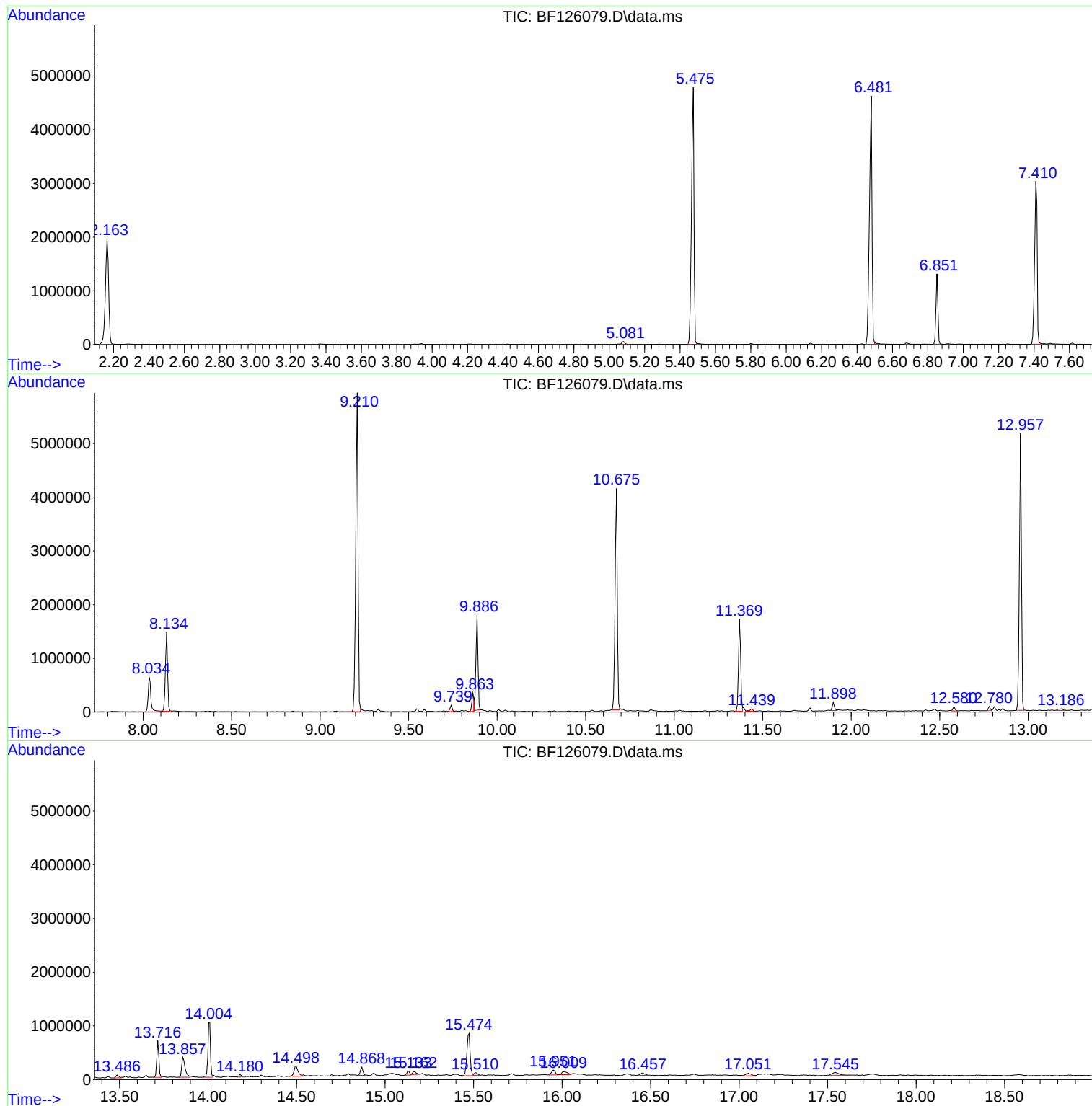
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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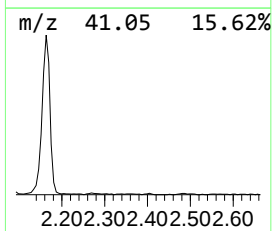
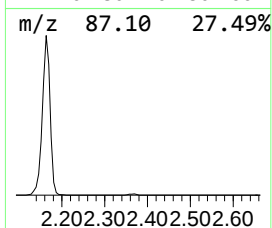
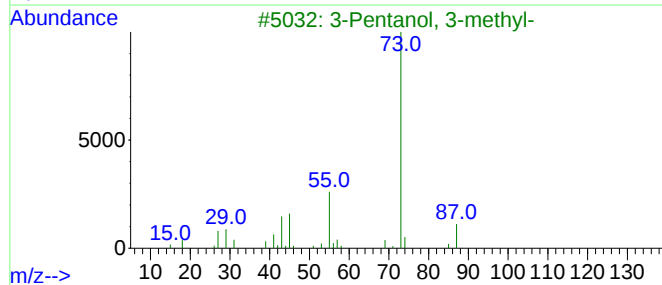
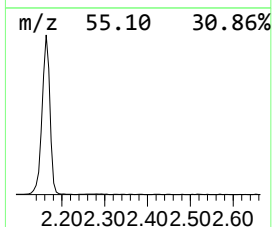
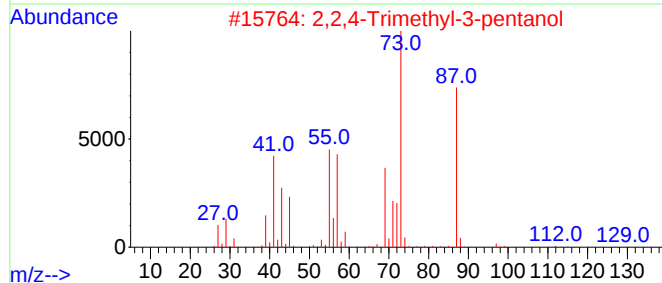
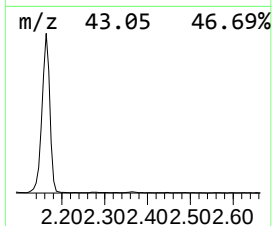
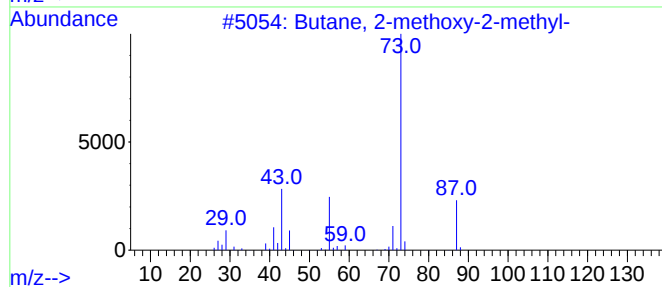
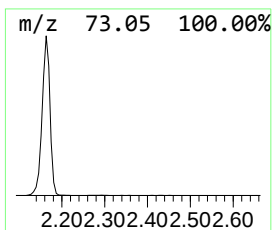
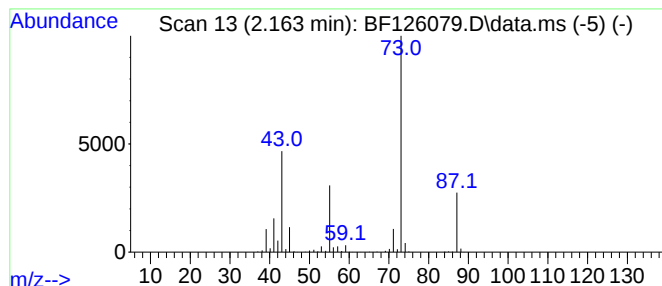
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	50.40 ng	2485440	1,4-Dichlorobenzene-d4	6.851

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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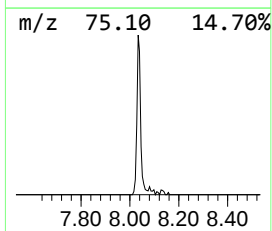
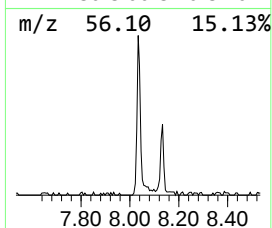
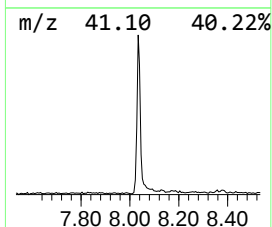
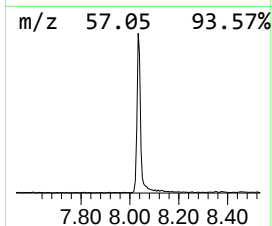
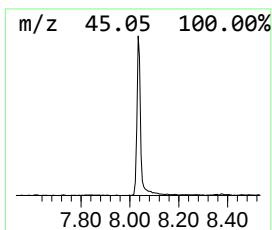
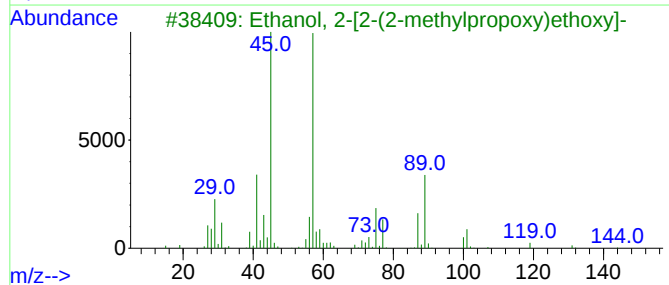
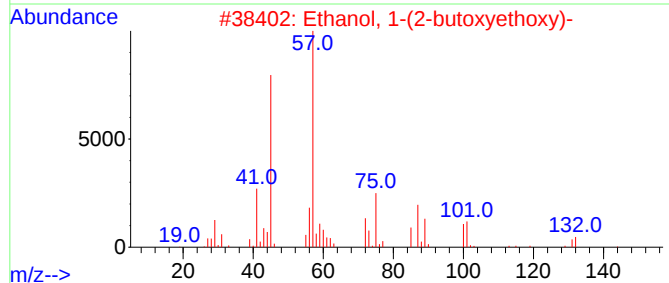
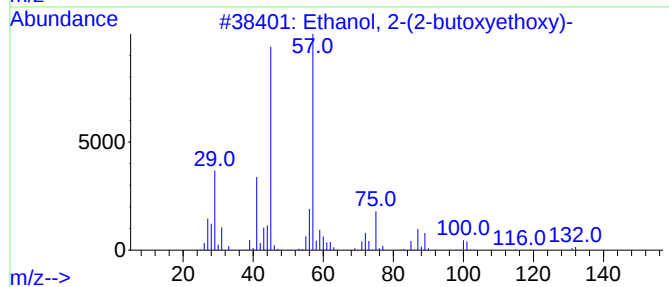
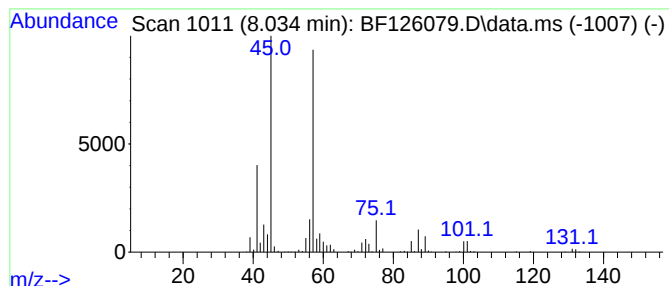
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	11.03 ng	690177	Naphthalene-d8	8.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	47



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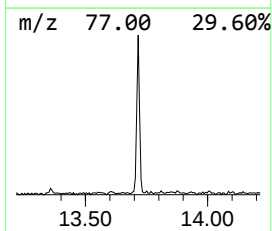
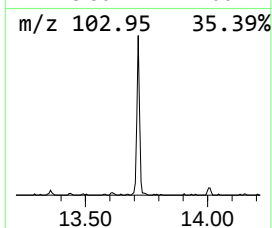
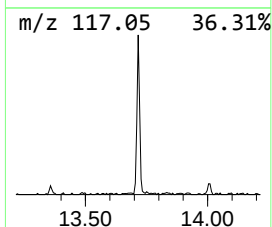
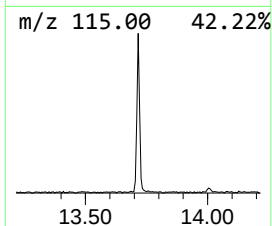
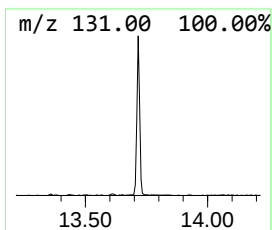
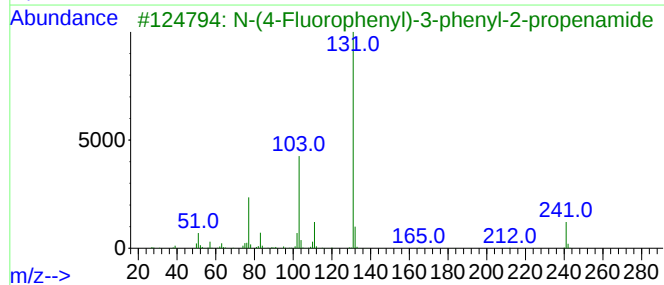
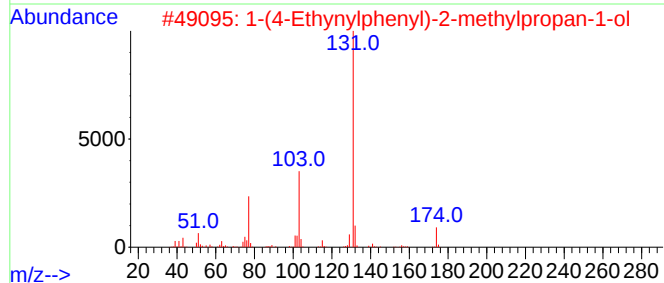
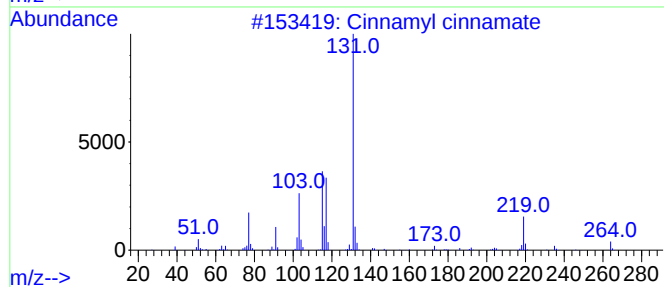
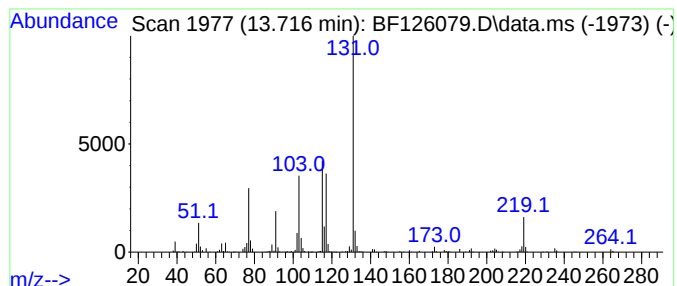
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.716	10.95 ng	555192	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			1-(4-Ethynylphenyl)-2-methylprop...	174	C12H14O	1000466-39-4	47
3			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47
4			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	47
5			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47



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Instrument :
BNA_F
ClientSampleId :
TP-5

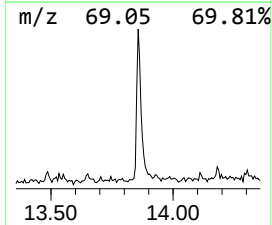
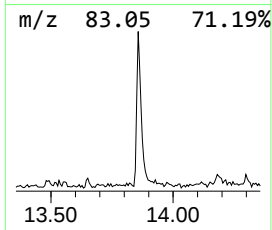
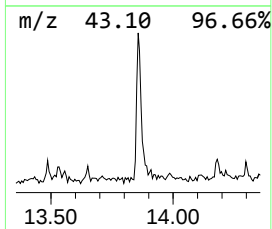
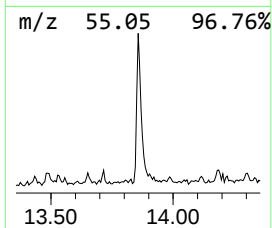
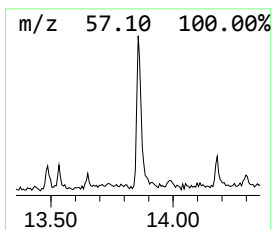
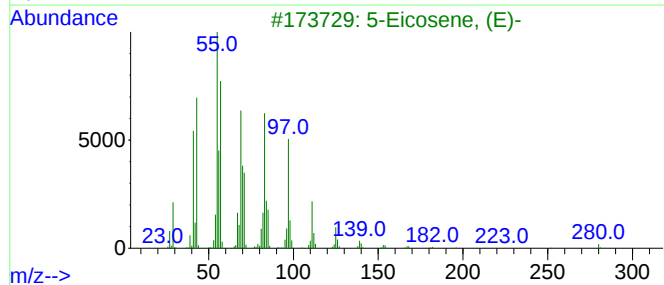
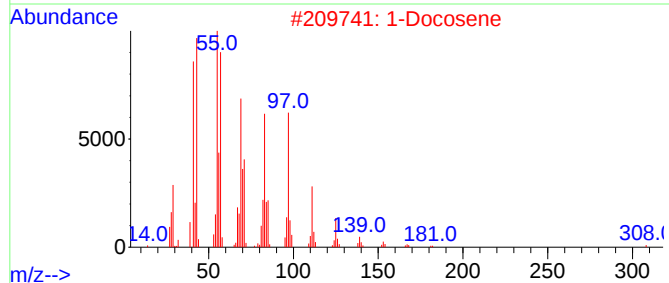
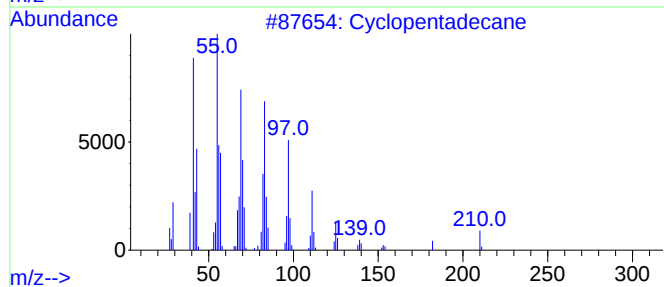
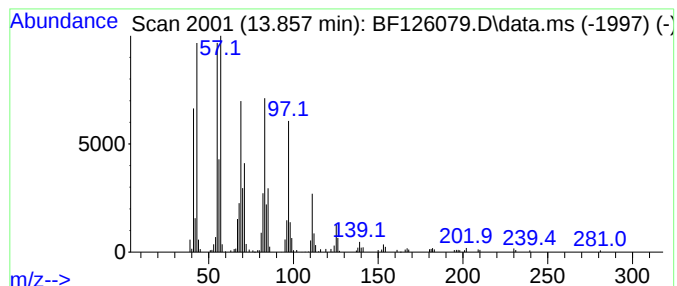
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	9.65 ng	489295	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			1-Docosene	308	C22H44	001599-67-3	94
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



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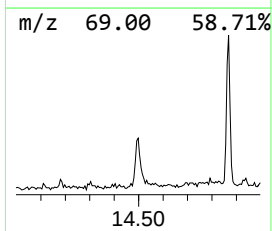
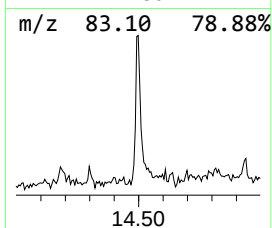
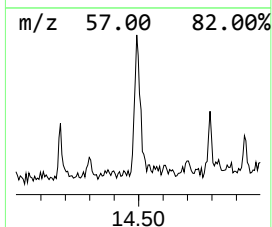
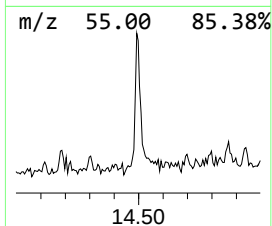
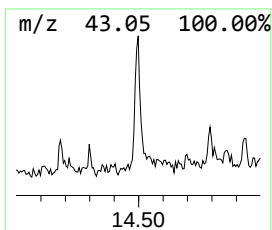
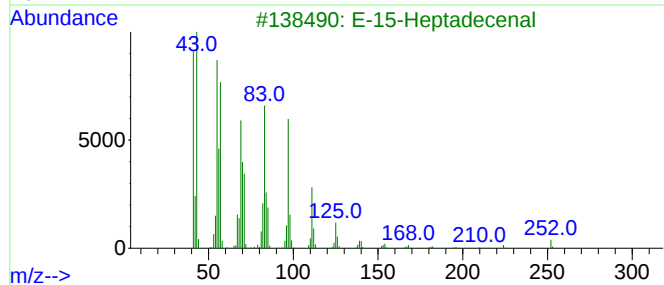
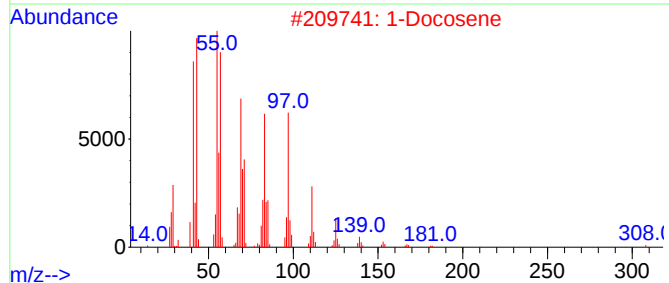
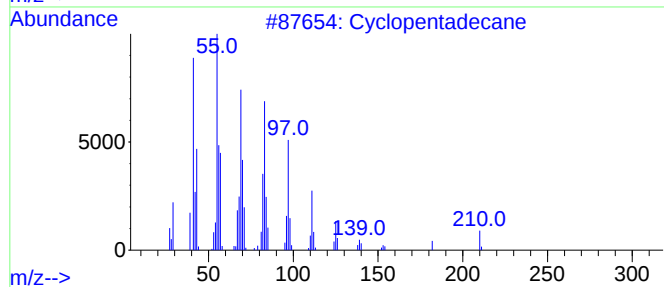
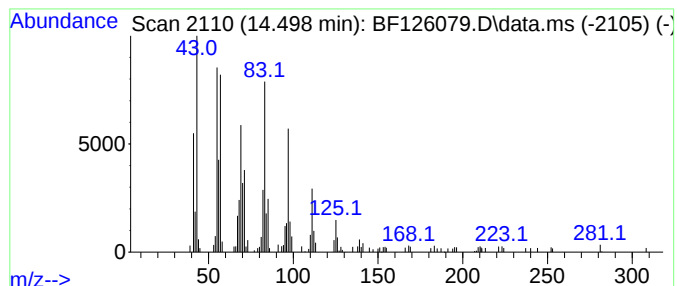
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.498	5.93 ng	300918	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	1-Docosene	308	C22H44	001599-67-3	95
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126079.D
Acq On : 9 Nov 2021 13:13
Operator : JU/CG
Sample : M4540-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

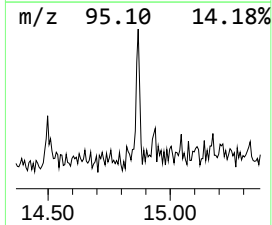
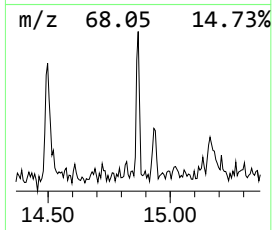
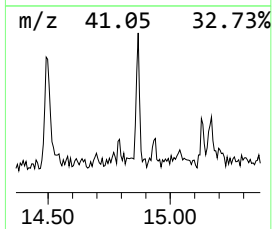
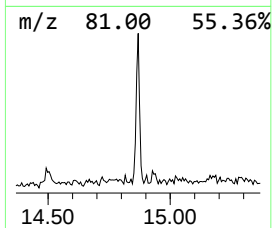
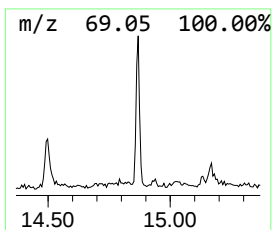
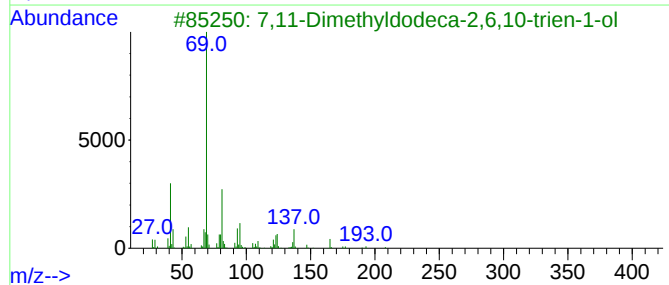
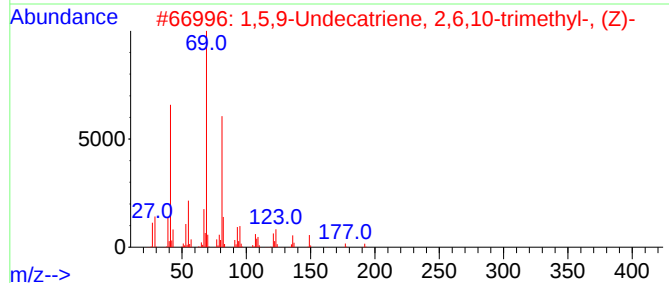
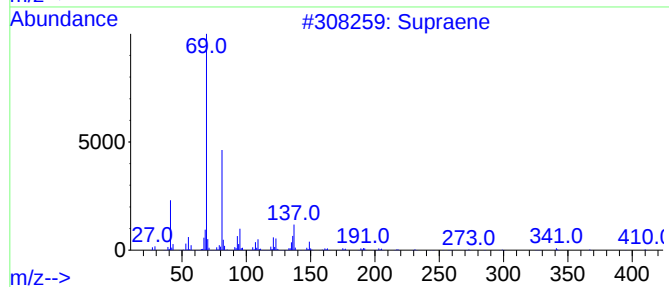
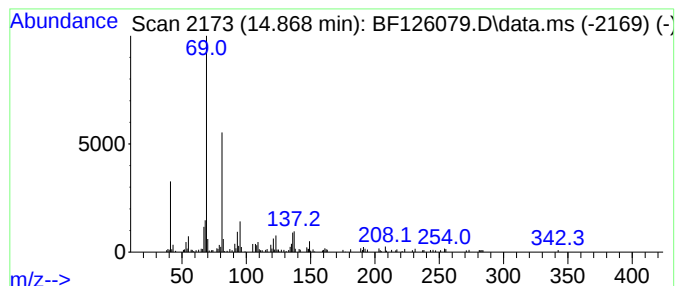
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.98 ng	149900	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4			3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126079.D
Acq On : 9 Nov 2021 13:13
Operator : JU/CG
Sample : M4540-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

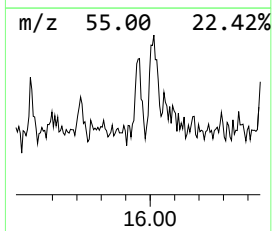
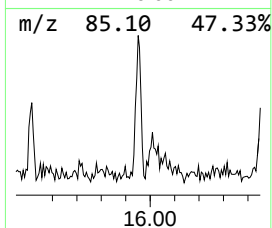
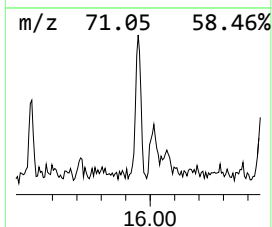
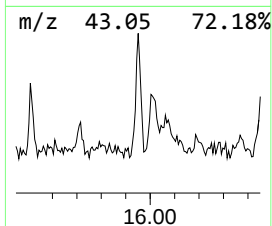
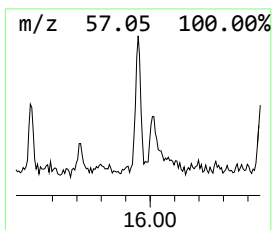
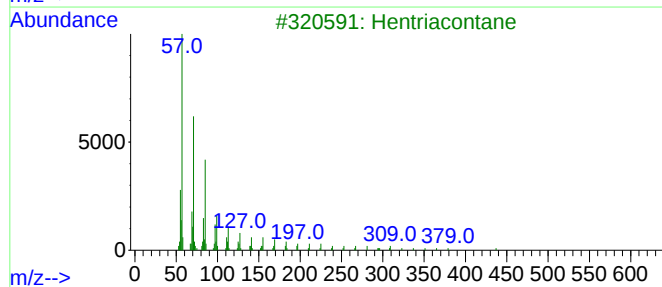
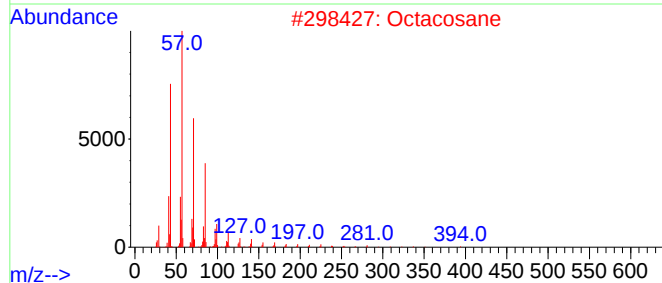
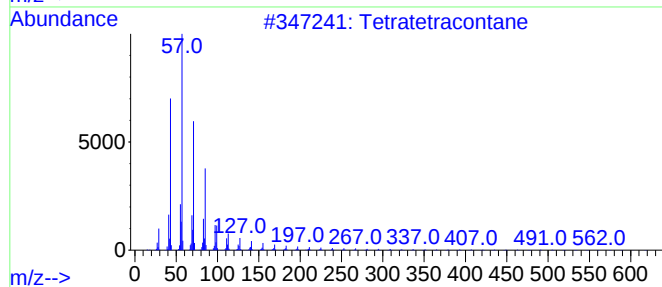
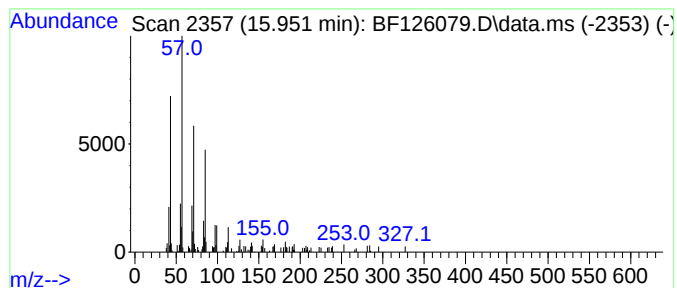
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.47 ng	124238	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126079.D
Acq On : 9 Nov 2021 13:13
Operator : JU/CG
Sample : M4540-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

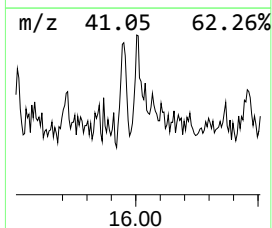
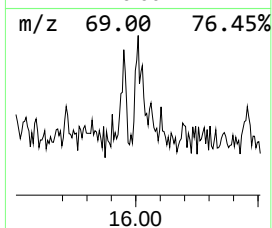
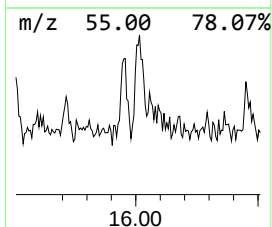
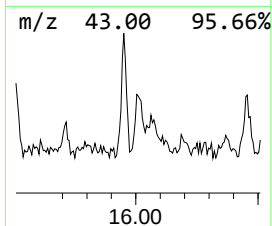
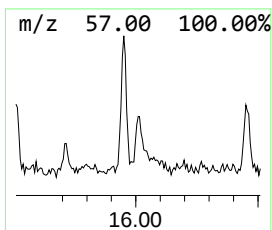
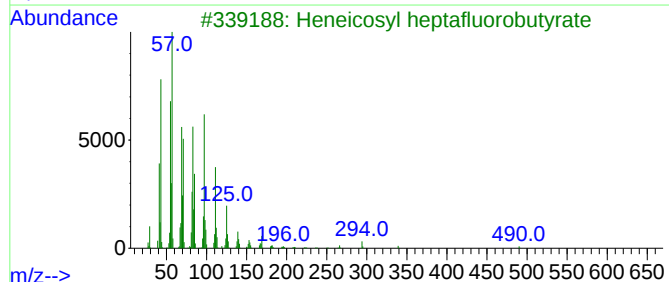
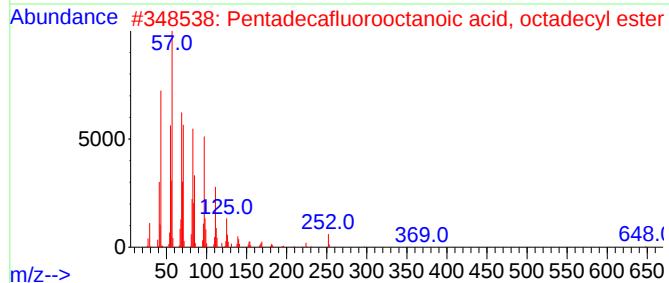
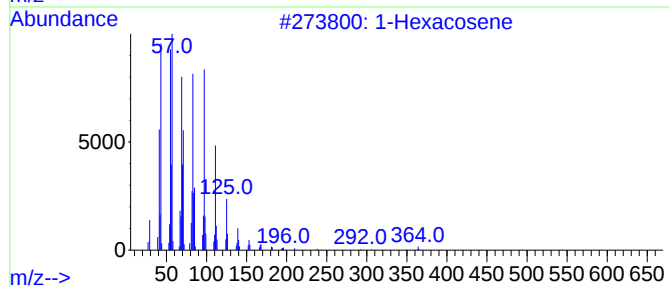
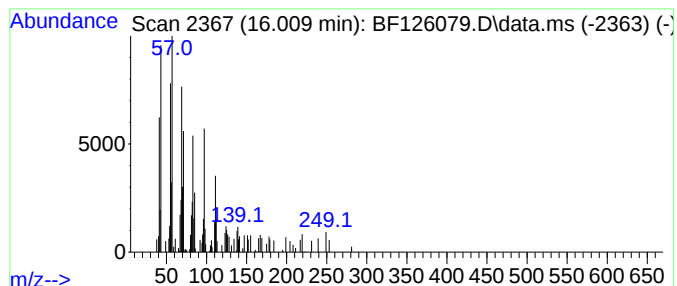
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexacosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.57 ng	129517	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	83
2	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	64
3	Heneicosyl heptafluorobutyrate			508	C25H43F7O2	1000351-83-8	60
4	Tricosyl pentafluoropropionate			486	C26H47F5O2	1000351-81-0	60
5	Octacosyl heptafluorobutyrate			606	C32H57F7O2	1010351-83-6	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126079.D
Acq On : 9 Nov 2021 13:13
Operator : JU/CG
Sample : M4540-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

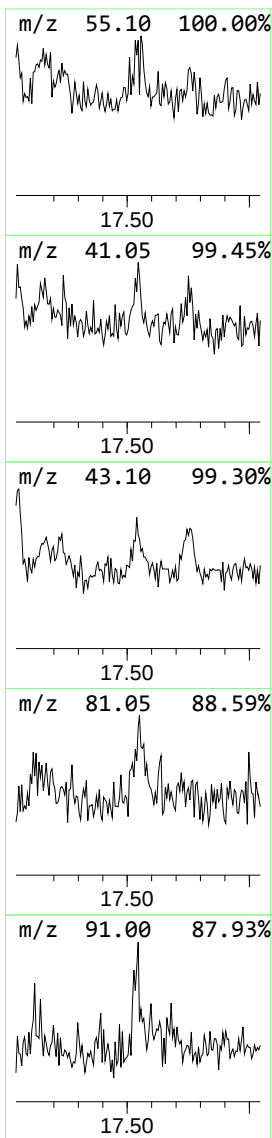
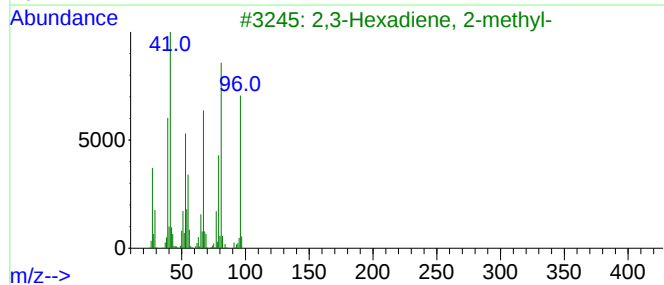
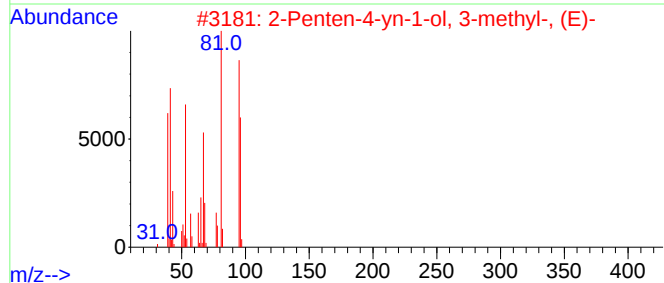
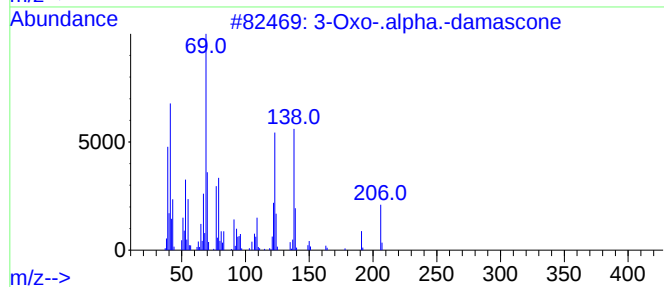
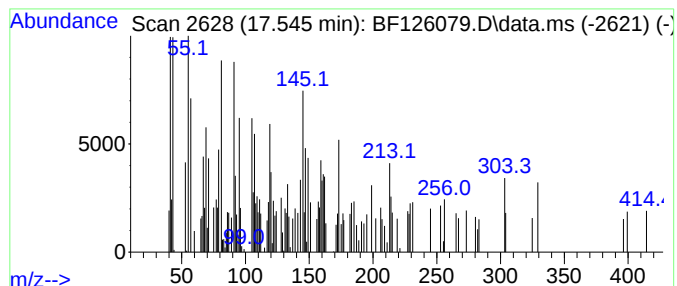
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.545 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.545	2.96 ng	149238	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Oxo-.alpha.-damascone	206	C13H18O2	053398-09-7	27
2			2-Penten-4-yn-1-ol, 3-methyl-, (E)-	96	C6H8O	006153-06-6	25
3			2,3-Hexadiene, 2-methyl-	96	C7H12	029212-09-7	25
4			1-Methyl-5-[1-(2,4-dinitrophenyl)...]	304	C13H12N4O5	100725-19-7	22
5			Formaldehyde, methyl(2-propynyl)...	96	C5H8N2	110213-10-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126079.D
Acq On : 9 Nov 2021 13:13
Operator : JU/CG
Sample : M4540-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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...	2.163	50.4	ng	2485440	1	6.851	986215	20.0
Ethanol, 2-(2-b...	8.034	11.0	ng	690177	2	8.134	1251260	20.0
Cinnamyl cinnamate	13.716	10.9	ng	555192	5	14.010	1014280	20.0
Cyclopentadecane	13.857	9.7	ng	489295	5	14.010	1014280	20.0
1-Docosene	14.498	5.9	ng	300918	5	14.010	1014280	20.0
Supraene	14.868	3.0	ng	149900	6	15.474	1006830	20.0
Tetratetracontane	15.951	2.5	ng	124238	6	15.474	1006830	20.0
1-Hexacosene	16.009	2.6	ng	129517	6	15.474	1006830	20.0
unknown17.545	17.545	3.0	ng	149238	6	15.474	1006830	20.0