

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
 Data File : BF122155.D
 Acq On : 28 Oct 2020 19:02
 Operator : JU/CG
 Sample : L4526-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-225

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.339	550	553	580	rBV	1673537	2065750	94.91%	12.377%
2	6.369	725	728	756	rBV	1867341	2176475	100.00%	13.041%
3	6.581	761	764	784	rVV	25490	80524	3.70%	0.482%
4	6.716	784	787	798	rVB	610904	590045	27.11%	3.535%
5	7.286	880	884	909	rBV	1227638	1335190	61.35%	8.000%
6	7.998	1002	1005	1013	rBV	804545	715941	32.89%	4.290%
7	8.586	1101	1105	1109	rBV	39004	35012	1.61%	0.210%
8	9.069	1183	1187	1196	rVB	2323401	2061841	94.73%	12.354%
9	9.145	1197	1200	1204	rVB2	29452	27644	1.27%	0.166%
10	9.469	1252	1255	1260	rBV	314411	276679	12.71%	1.658%
11	9.610	1276	1279	1281	rBV3	25540	33109	1.52%	0.198%
12	9.651	1283	1286	1288	rVB2	36255	31765	1.46%	0.190%
13	9.692	1288	1293	1294	rBV4	31016	48378	2.22%	0.290%
14	9.745	1299	1302	1306	rVV	922006	816433	37.51%	4.892%
15	10.145	1368	1370	1373	rBV2	57056	43925	2.02%	0.263%
16	10.539	1434	1437	1442	rBV	802891	928846	42.68%	5.565%
17	10.657	1455	1457	1460	rVB	104624	94593	4.35%	0.567%
18	11.121	1534	1536	1541	rVB	165021	178393	8.20%	1.069%
19	11.233	1552	1555	1559	rBV	812812	819699	37.66%	4.911%
20	12.268	1729	1731	1734	rVB	177243	152634	7.01%	0.915%
21	12.815	1821	1824	1831	rVB	1675919	1614371	74.17%	9.673%
22	13.715	1974	1977	1996	rVB3	148038	405183	18.62%	2.428%
23	13.880	2001	2005	2013	rVB	593216	633168	29.09%	3.794%
24	14.368	2084	2088	2095	rVB5	50162	90959	4.18%	0.545%
25	14.627	2129	2132	2138	rVV6	21529	34269	1.57%	0.205%
26	14.692	2141	2143	2148	rVB2	36965	40685	1.87%	0.244%
27	14.762	2152	2155	2159	rVB	118329	112649	5.18%	0.675%
28	14.939	2182	2185	2189	rVB	101377	116943	5.37%	0.701%
29	14.998	2189	2195	2207	rVB4	64710	204060	9.38%	1.223%
30	15.309	2243	2248	2258	rVB	468860	614015	28.21%	3.679%
31	15.486	2274	2278	2284	rVB3	41619	54619	2.51%	0.327%
32	15.698	2310	2314	2320	rVB	83085	113798	5.23%	0.682%
33	16.439	2436	2440	2446	rVB4	23312	40686	1.87%	0.244%
34	16.709	2483	2486	2492	rVB2	25866	37923	1.74%	0.227%
35	16.945	2523	2526	2532	rVB4	25116	38883	1.79%	0.233%
36	17.345	2590	2594	2599	rVB6	12896	24608	1.13%	0.147%

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

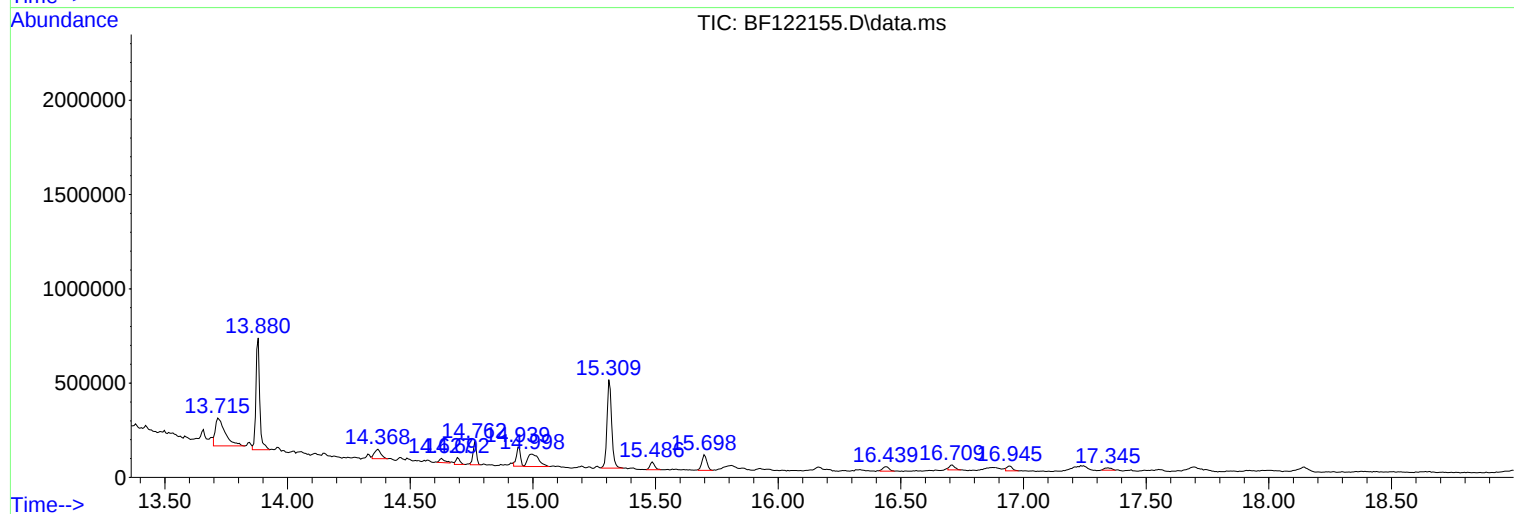
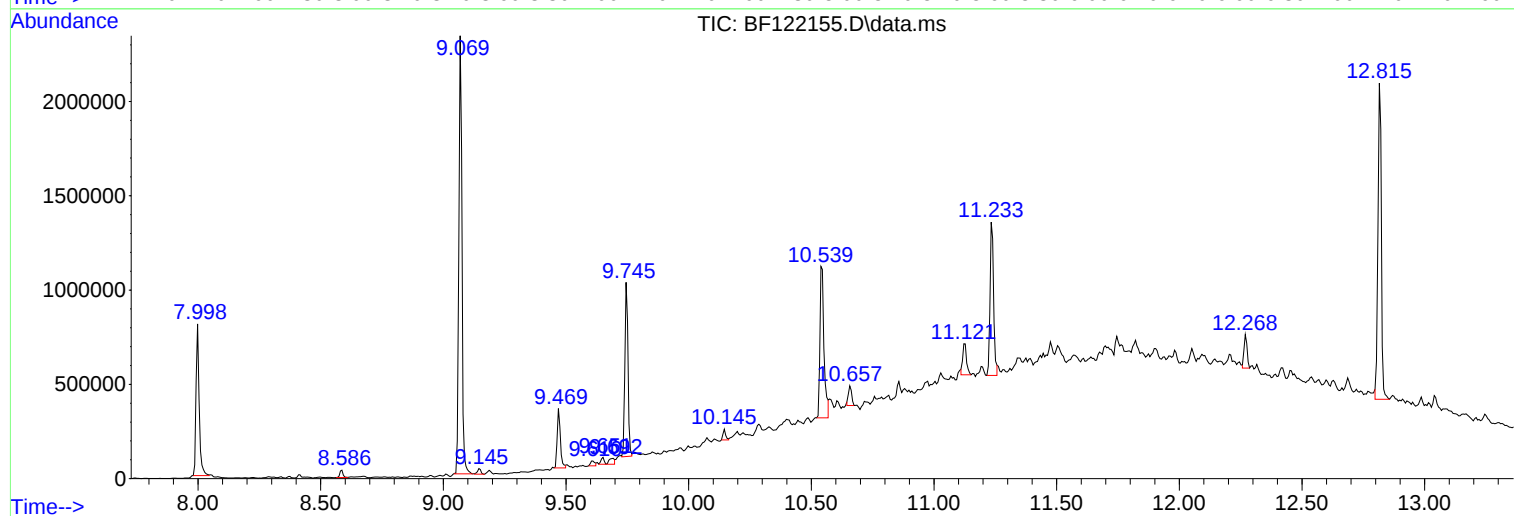
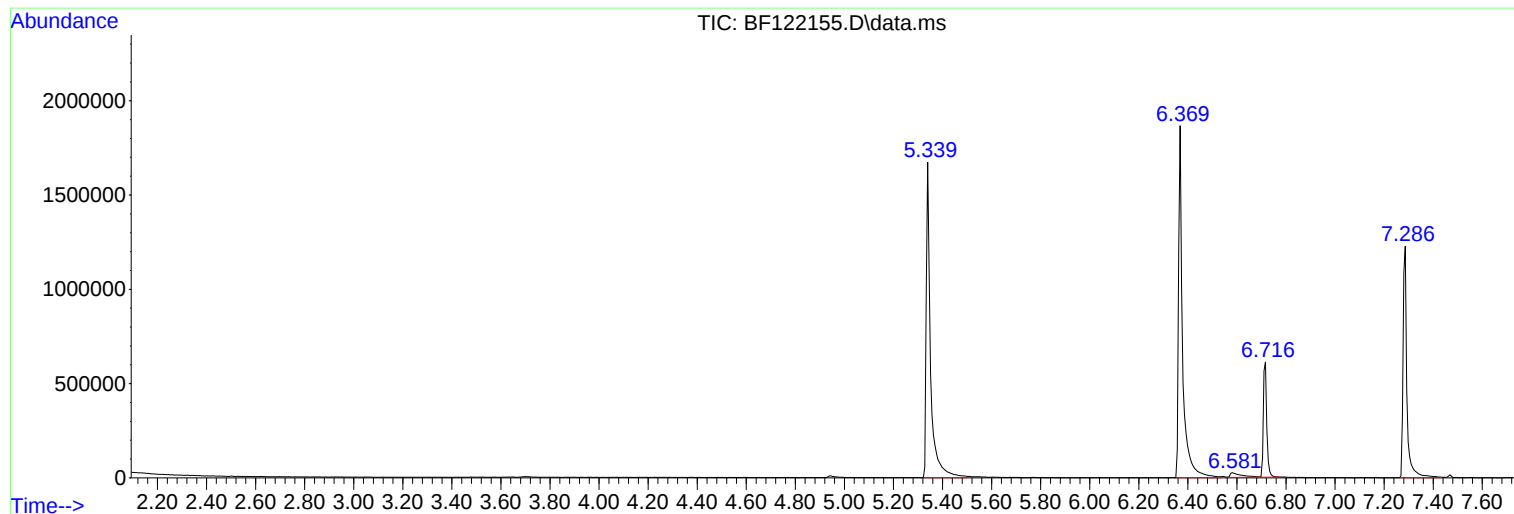
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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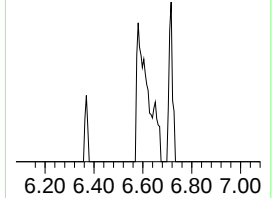
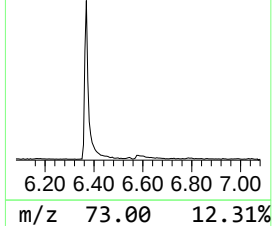
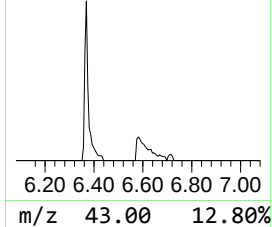
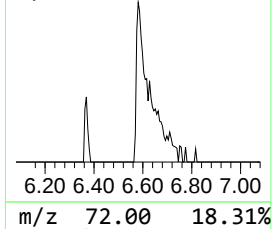
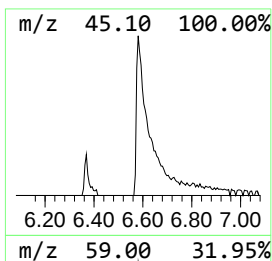
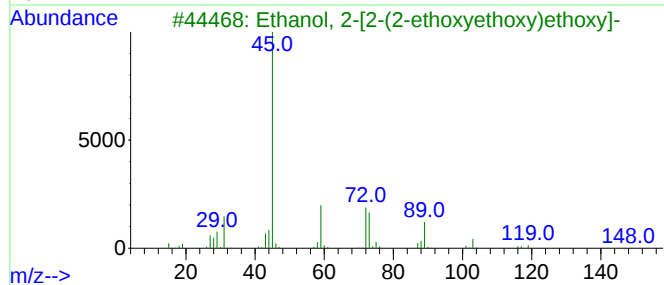
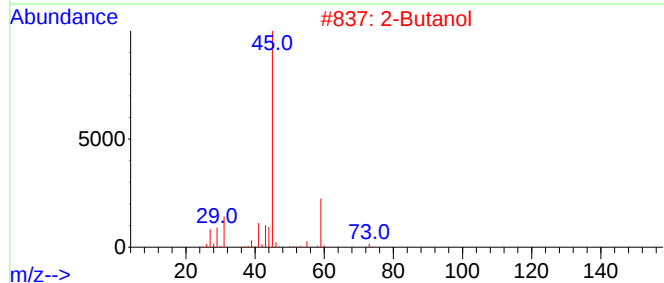
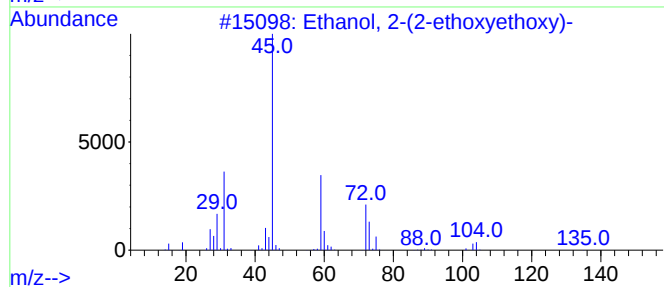
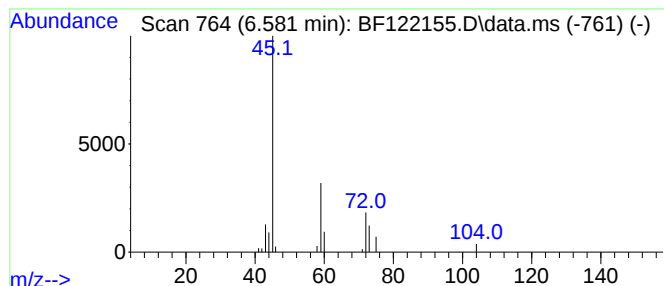
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	2.73 ng	80524	1,4-Dichlorobenzene-d4	6.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2			2-Butanol	74	C4H10O	000078-92-2	45
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39
5			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	38



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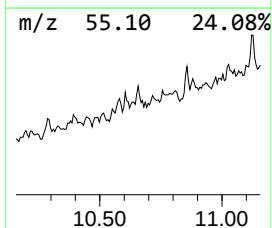
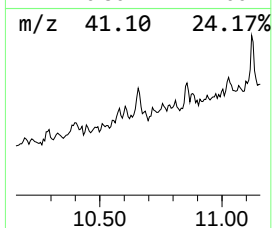
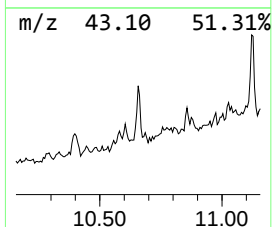
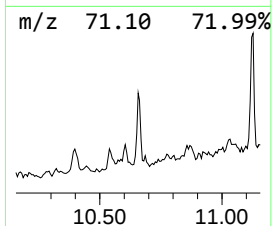
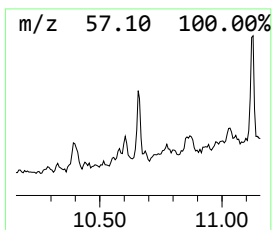
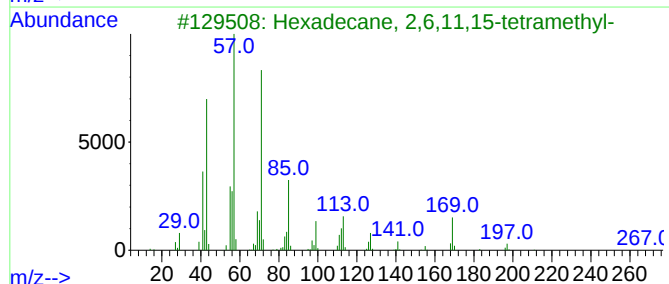
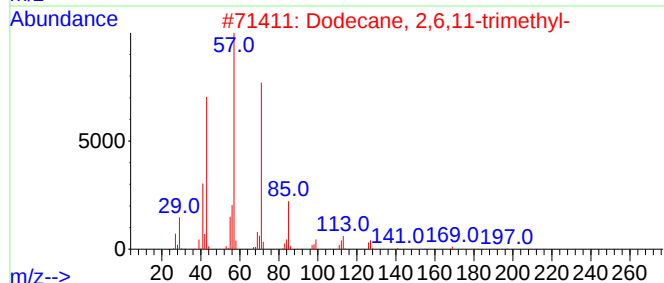
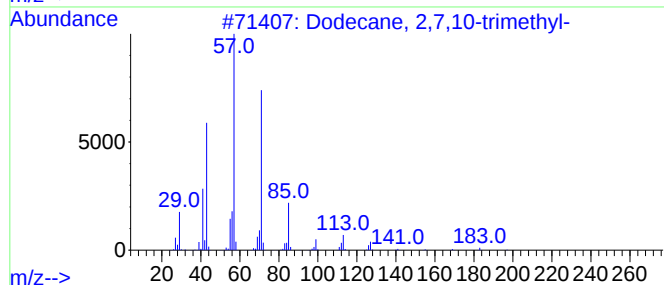
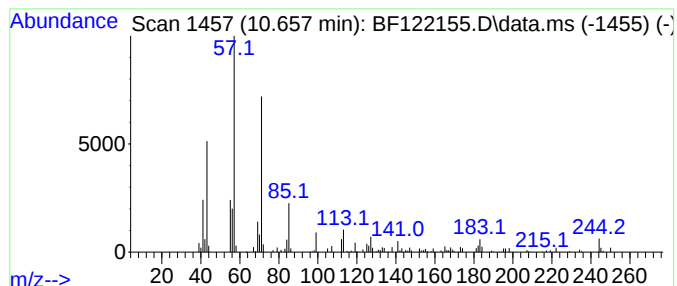
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 2,7,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	2.31 ng	94593	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	74
4			Octane, 2-methyl-	128	C9H20	003221-61-2	64
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	59



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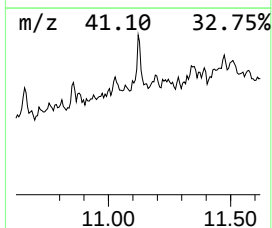
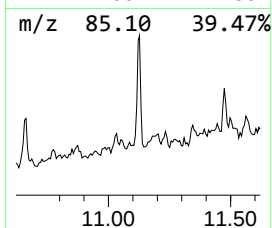
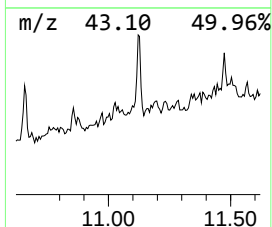
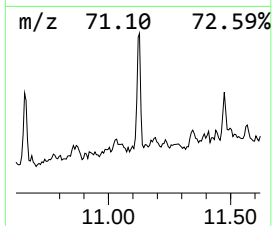
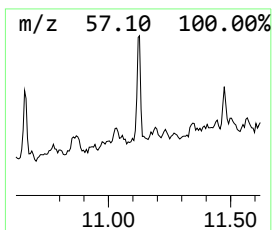
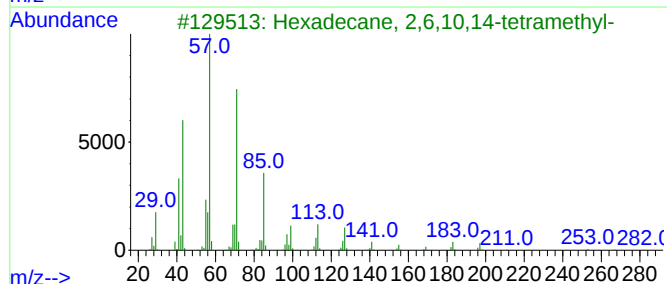
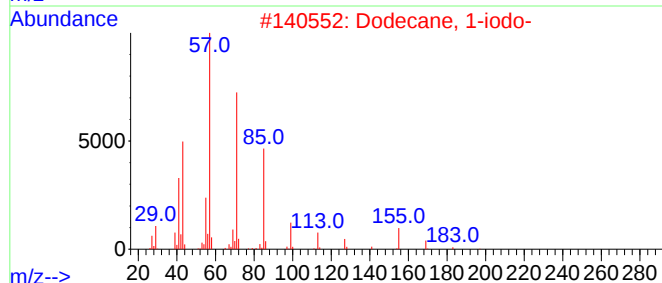
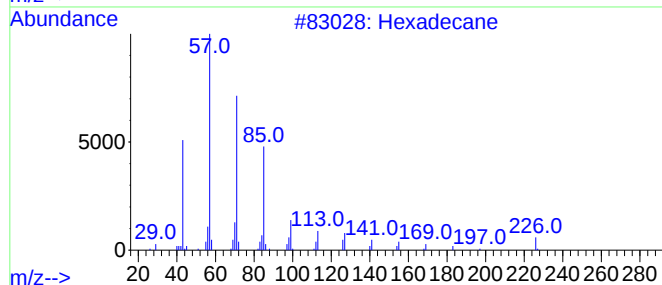
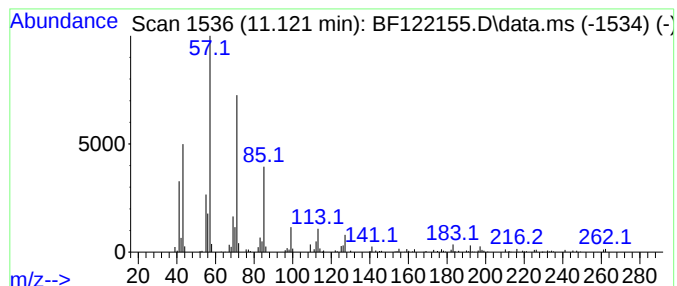
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.121	4.35 ng	178393	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	87
2			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	78
5			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	78



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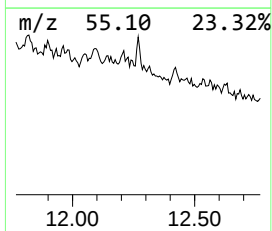
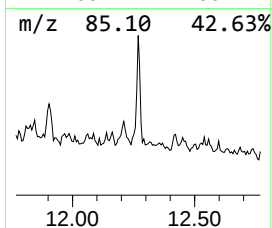
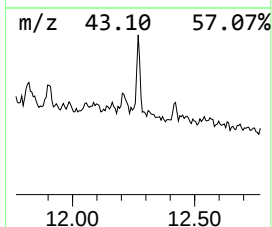
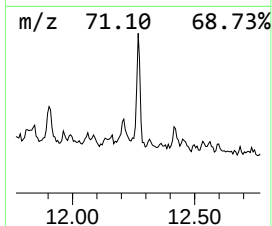
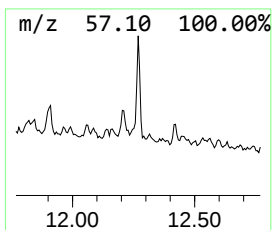
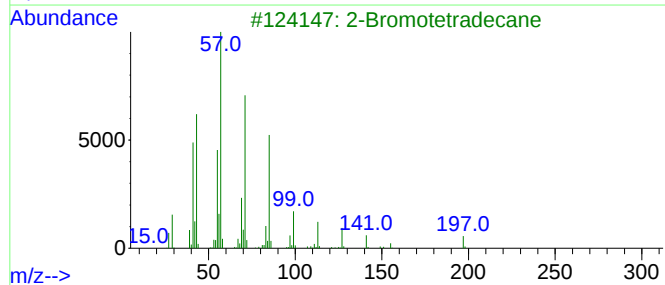
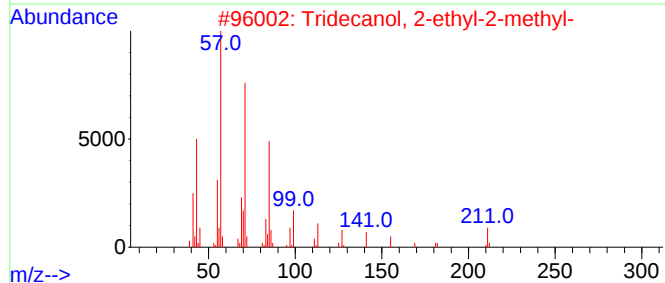
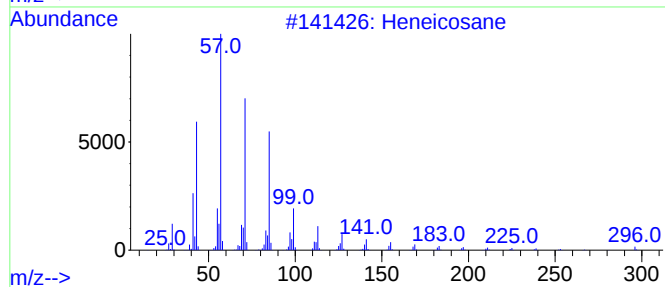
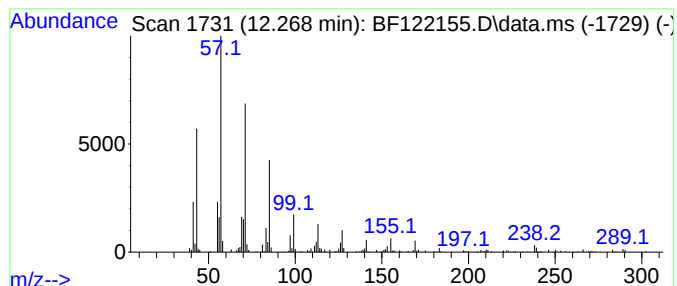
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.268	3.72 ng	152634	Phenanthrene-d10	11.233	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Pentacosane	352	C25H52	000629-99-2	87



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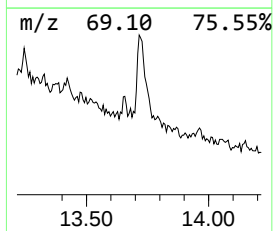
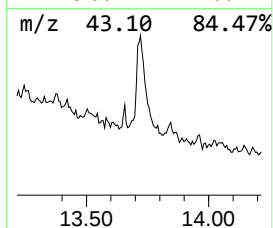
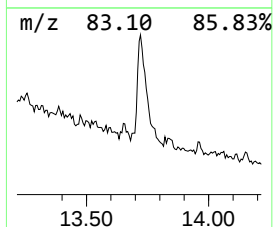
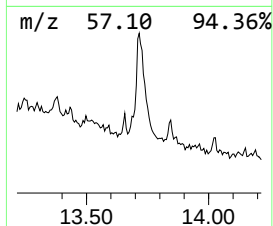
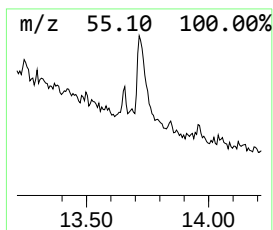
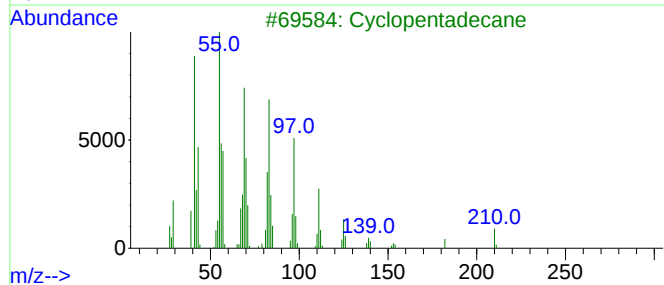
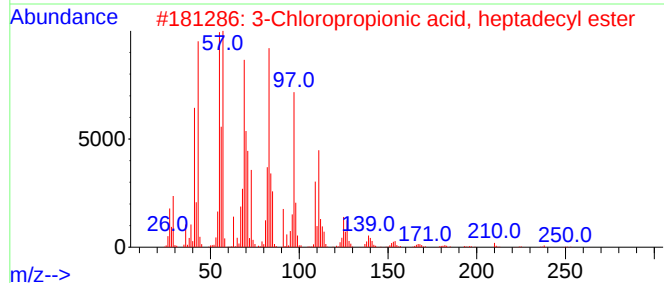
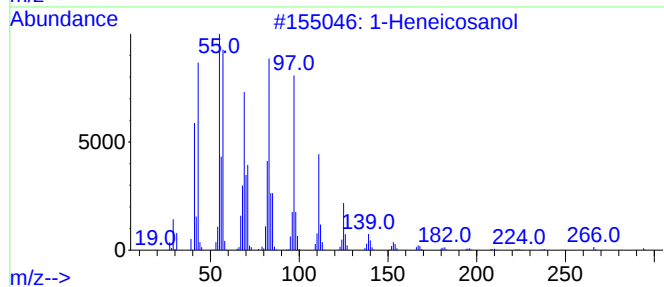
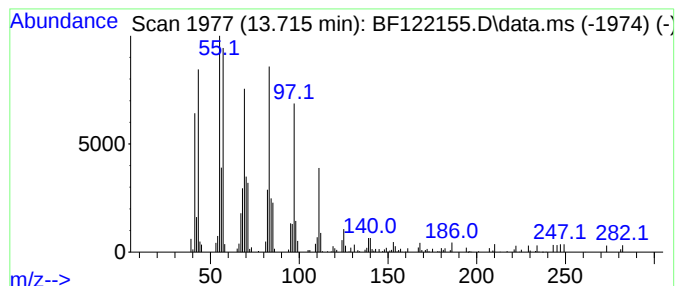
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.715	12.80 ng	405183	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3			Cyclopentadecane	210	C15H30	000295-48-7	91
4			1-Hexadecanol	242	C16H34O	036653-82-4	90
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
Data File : BF122155.D
Acq On : 28 Oct 2020 19:02
Operator : JU/CG
Sample : L4526-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-225

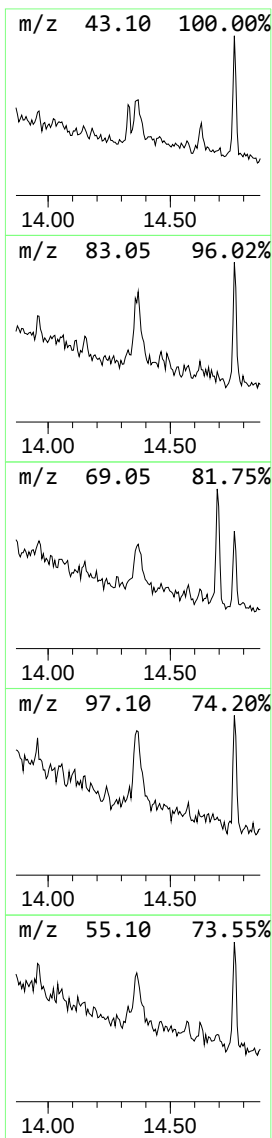
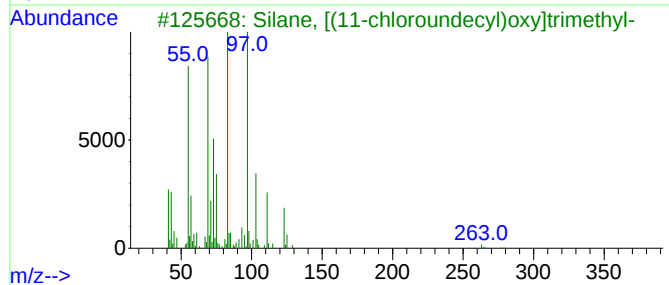
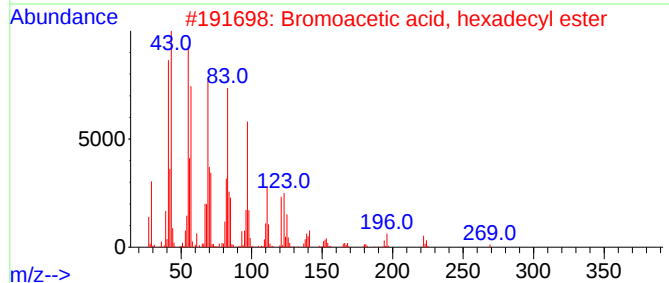
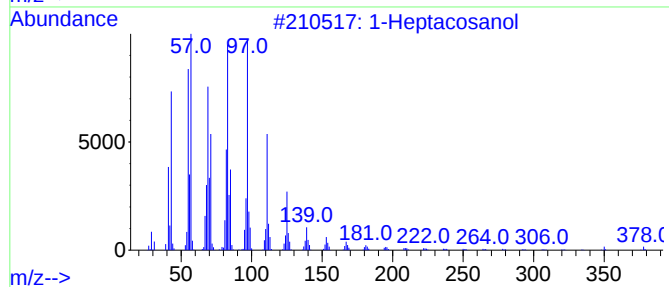
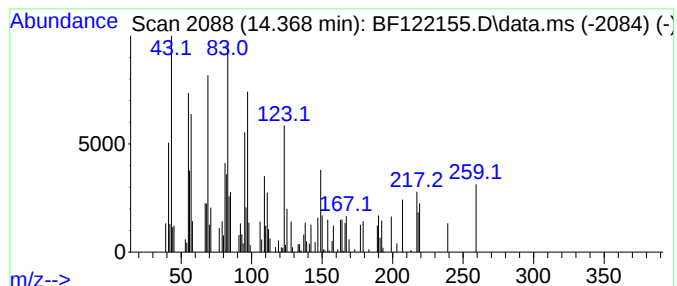
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	2.87 ng	90959	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	49
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	49
3			Silane, [(11-chloroundecyl)oxy]t...	278	C14H31ClOSi	026305-82-8	47
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	43
5			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
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Acq On : 28 Oct 2020 19:02
Operator : JU/CG
Sample : L4526-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

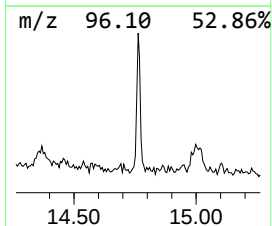
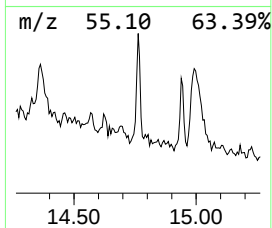
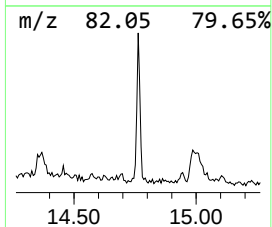
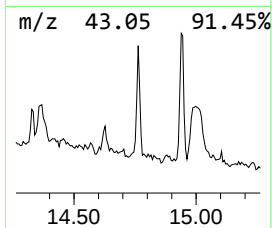
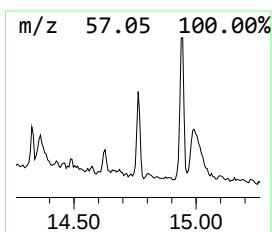
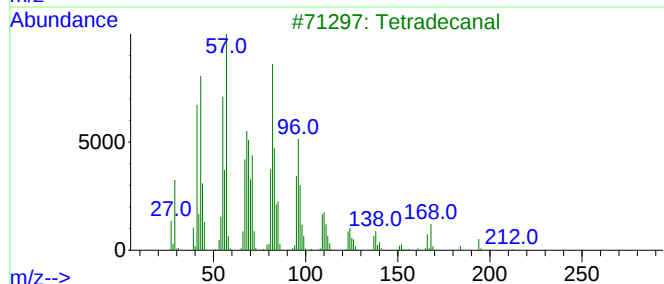
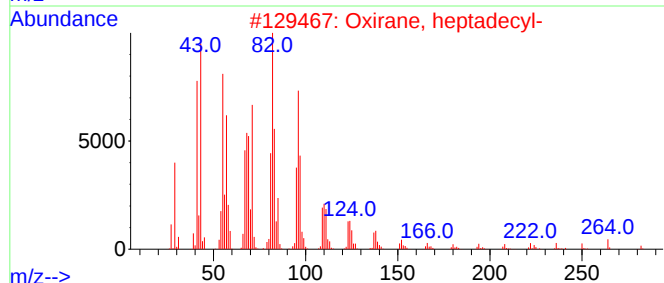
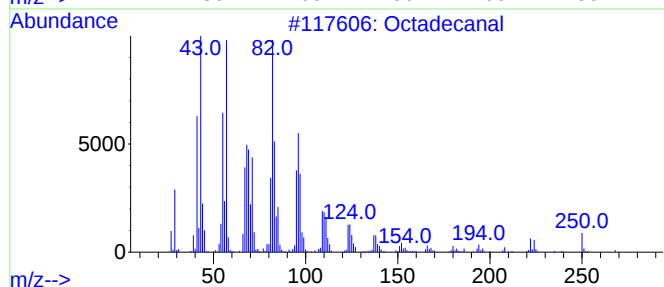
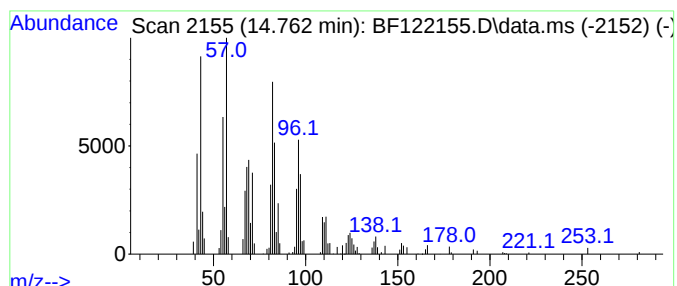
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.762	3.67 ng	112649	Perylene-d12	15.309	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Tetradecanal	212	C14H28O	000124-25-4	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5	1,19-Eicosadiene	278	C20H38	014811-95-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
Data File : BF122155.D
Acq On : 28 Oct 2020 19:02
Operator : JU/CG
Sample : L4526-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-225

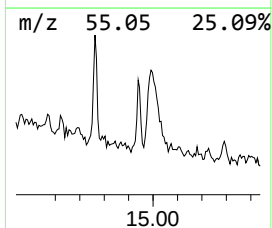
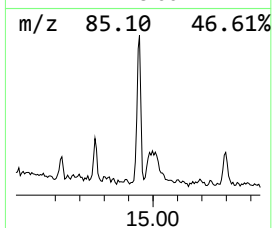
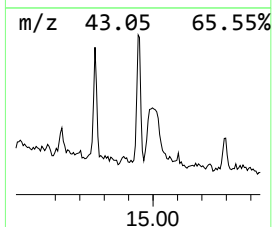
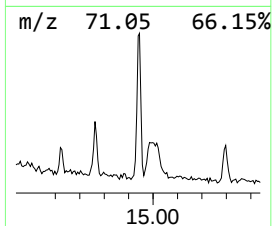
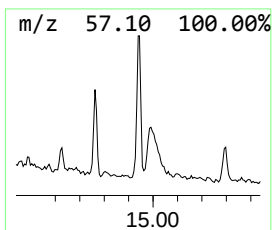
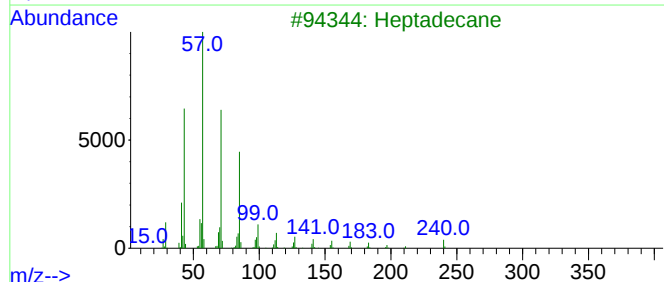
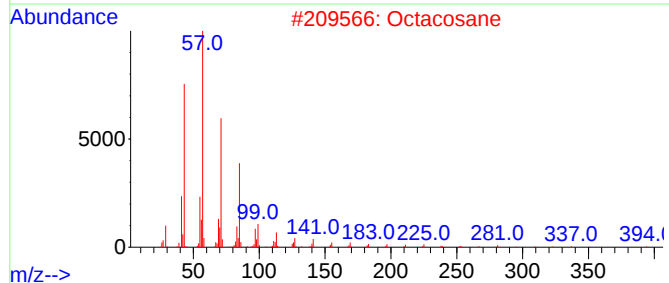
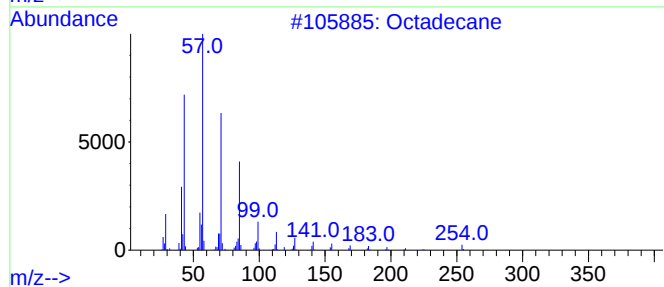
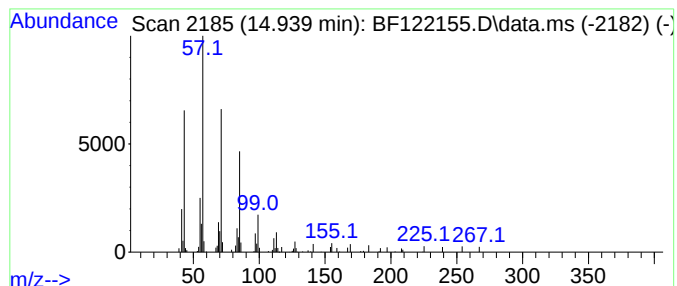
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	3.81 ng	116943	Perylene-d12	15.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
Data File : BF122155.D
Acq On : 28 Oct 2020 19:02
Operator : JU/CG
Sample : L4526-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

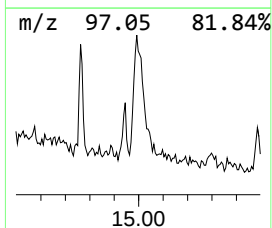
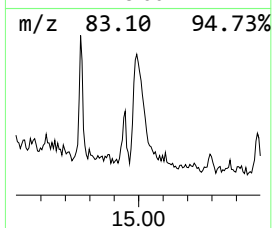
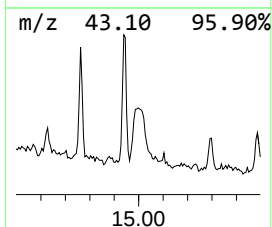
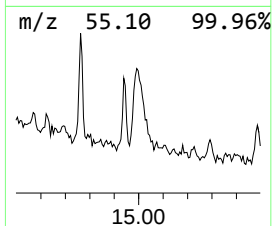
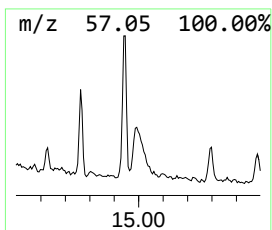
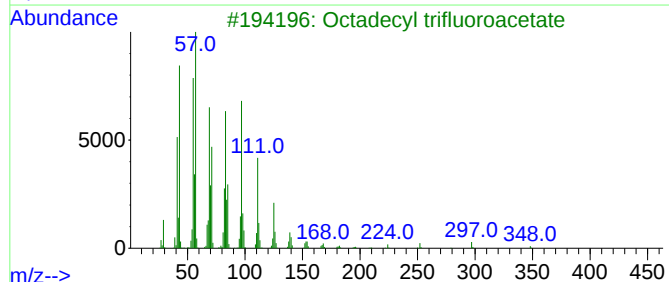
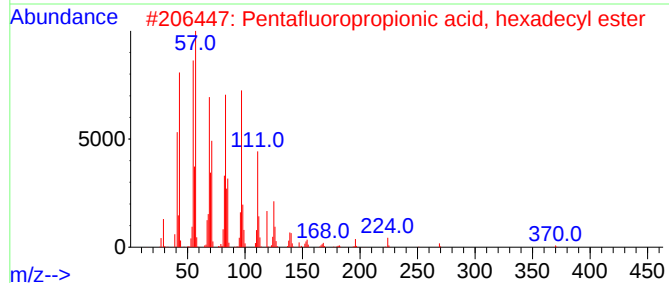
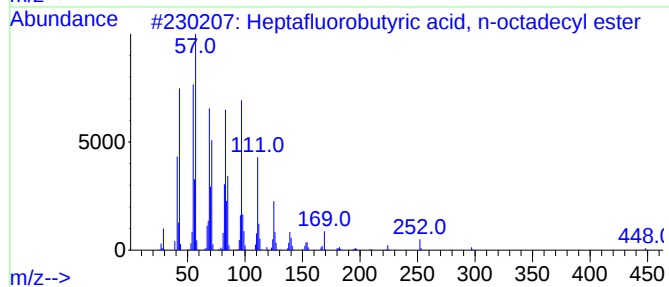
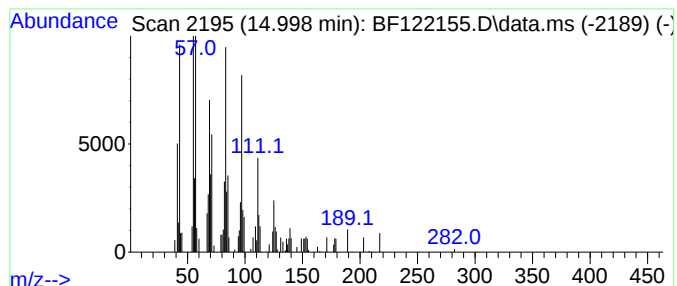
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.998	6.65 ng	204060	Perylene-d12	15.309	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	95
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	95
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	93
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
Data File : BF122155.D
Acq On : 28 Oct 2020 19:02
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Sample : L4526-01
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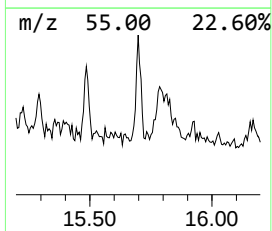
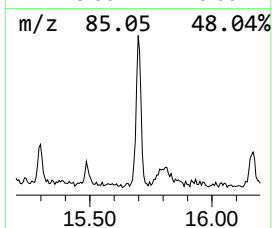
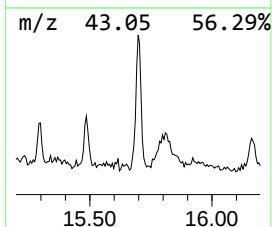
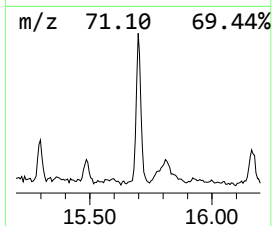
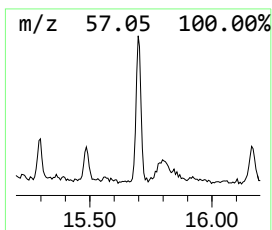
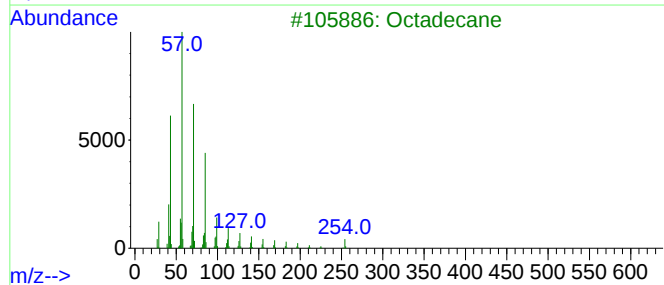
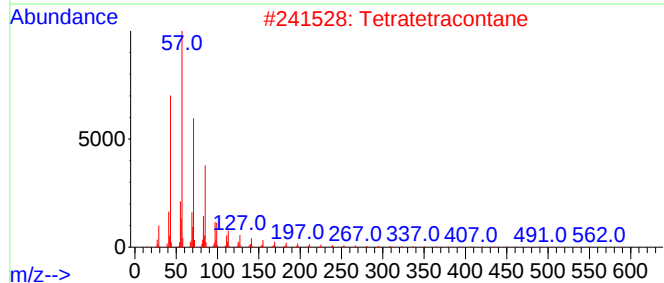
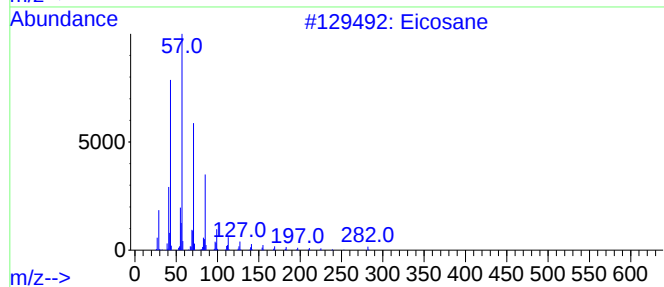
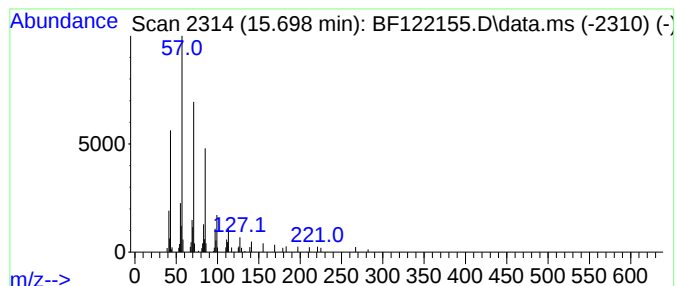
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.698	3.71 ng	113798	Perylene-d12	15.309	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Octadecane	254	C18H38	000593-45-3	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102820\
Data File : BF122155.D
Acq On : 28 Oct 2020 19:02
Operator : JU/CG
Sample : L4526-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Dodecane, 2,7,1...	10.657	2.3	ng	94593	4	11.233	819699	20.0
Hexadecane	11.121	4.3	ng	178393	4	11.233	819699	20.0
Heneicosane	12.268	3.7	ng	152634	4	11.233	819699	20.0
1-Heneicosanol	13.715	12.8	ng	405183	5	13.880	633168	20.0
1-Heptacosanol	14.368	2.9	ng	90959	5	13.880	633168	20.0
Octadecanal	14.762	3.7	ng	112649	6	15.309	614015	20.0
Octadecane	14.939	3.8	ng	116943	6	15.309	614015	20.0
Heptafluorobuty...	14.998	6.7	ng	204060	6	15.309	614015	20.0
Eicosane	15.698	3.7	ng	113798	6	15.309	614015	20.0