

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
 Data File : BF125346.D
 Acq On : 3 Sep 2021 14:58
 Operator : JU/CG
 Sample : M3606-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BPU-BFD

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	12	20	30	rVB	3426360	4839462	86.03%	12.441%
2	5.116	512	515	525	rVB	55914	68020	1.21%	0.175%
3	5.516	579	583	587	rBV	2524343	2413270	42.90%	6.204%
4	6.522	750	754	766	rVB	1755860	1535040	27.29%	3.946%
5	6.898	814	818	821	rBV	1217047	987199	17.55%	2.538%
6	7.463	908	914	917	rBV	3123848	3226276	57.35%	8.294%
7	8.081	1015	1019	1032	rBV	1417699	1510807	26.86%	3.884%
8	8.181	1032	1036	1039	rVB	1515738	1273059	22.63%	3.273%
9	9.257	1213	1219	1222	rBV	6050011	5528398	98.28%	14.212%
10	9.363	1234	1237	1241	rBV	177928	179974	3.20%	0.463%
11	9.516	1259	1263	1268	rBV	80664	102547	1.82%	0.264%
12	9.592	1273	1276	1278	rBV	73724	70916	1.26%	0.182%
13	9.934	1330	1334	1338	rBV	1578638	1421117	25.26%	3.653%
14	10.034	1348	1351	1356	rVB	70123	88436	1.57%	0.227%
15	10.134	1363	1368	1372	rBV4	96827	117911	2.10%	0.303%
16	10.175	1372	1375	1384	rVB3	76403	93057	1.65%	0.239%
17	10.339	1399	1403	1409	rVB3	54798	104186	1.85%	0.268%
18	10.575	1441	1443	1449	rVB2	59431	78918	1.40%	0.203%
19	10.728	1464	1469	1472	rBV	3944620	3684707	65.50%	9.473%
20	10.845	1485	1489	1492	rBV	149362	124843	2.22%	0.321%
21	11.310	1564	1568	1574	rVB3	126738	153441	2.73%	0.394%
22	11.422	1583	1587	1590	rBV	1672531	1458388	25.93%	3.749%
23	11.804	1649	1652	1655	rVB	177961	154639	2.75%	0.398%
24	11.939	1670	1675	1680	rBV2	210863	293171	5.21%	0.754%
25	12.510	1767	1772	1778	rVB	510289	533423	9.48%	1.371%
26	12.598	1784	1787	1790	rBV	142559	112349	2.00%	0.289%
27	12.727	1806	1809	1817	rVB3	50533	67417	1.20%	0.173%
28	13.010	1852	1857	1860	rBV	5474001	5625366	100.00%	14.462%
29	13.569	1948	1952	1955	rBV2	80889	74803	1.33%	0.192%
30	13.857	1996	2001	2004	rBV	46656	65815	1.17%	0.169%
31	13.898	2004	2008	2010	rBV2	151908	148667	2.64%	0.382%
32	13.927	2010	2013	2019	rVB	182848	181539	3.23%	0.467%
33	14.063	2033	2036	2040	rVB	1278388	1078741	19.18%	2.773%
34	14.216	2058	2062	2065	rBV	118452	102609	1.82%	0.264%
35	14.521	2111	2114	2118	rVB	110295	92753	1.65%	0.238%
36	14.833	2163	2167	2171	rBV	94522	101684	1.81%	0.261%

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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-BF081821.M
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37	14.910	2177	2180	2185	rVB	83590	93589	1.66%	0.241%
38	15.180	2222	2226	2231	rBV	74534	85088	1.51%	0.219%
39	15.557	2285	2290	2301	rVB	782070	1026718	18.25%	2.639%

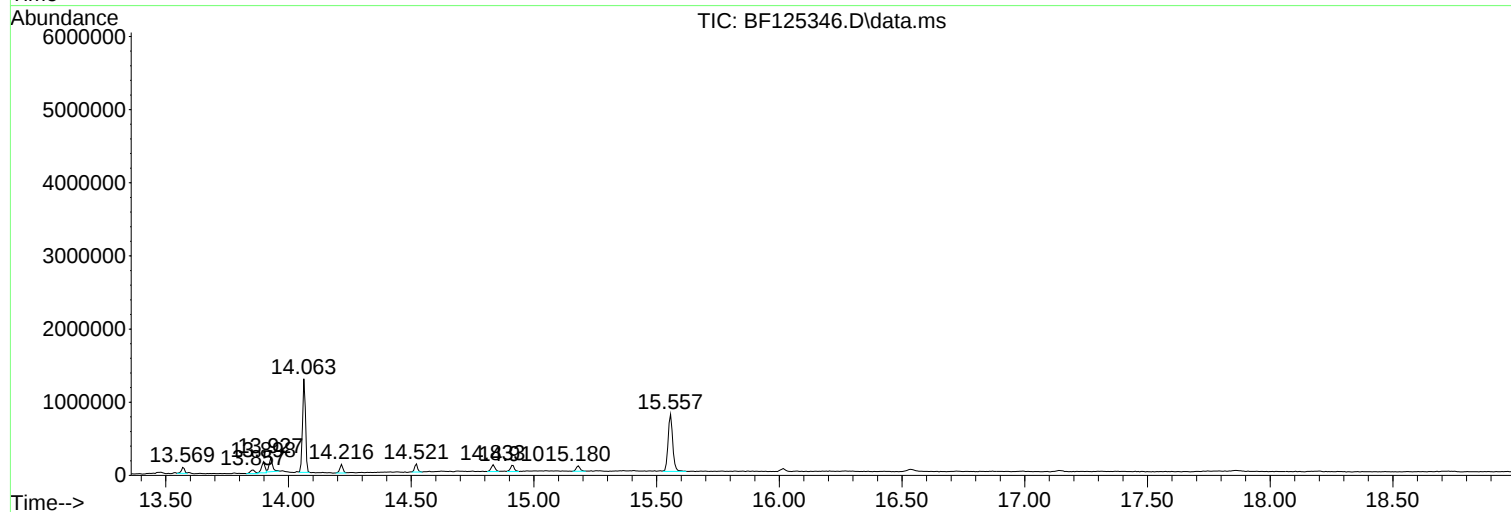
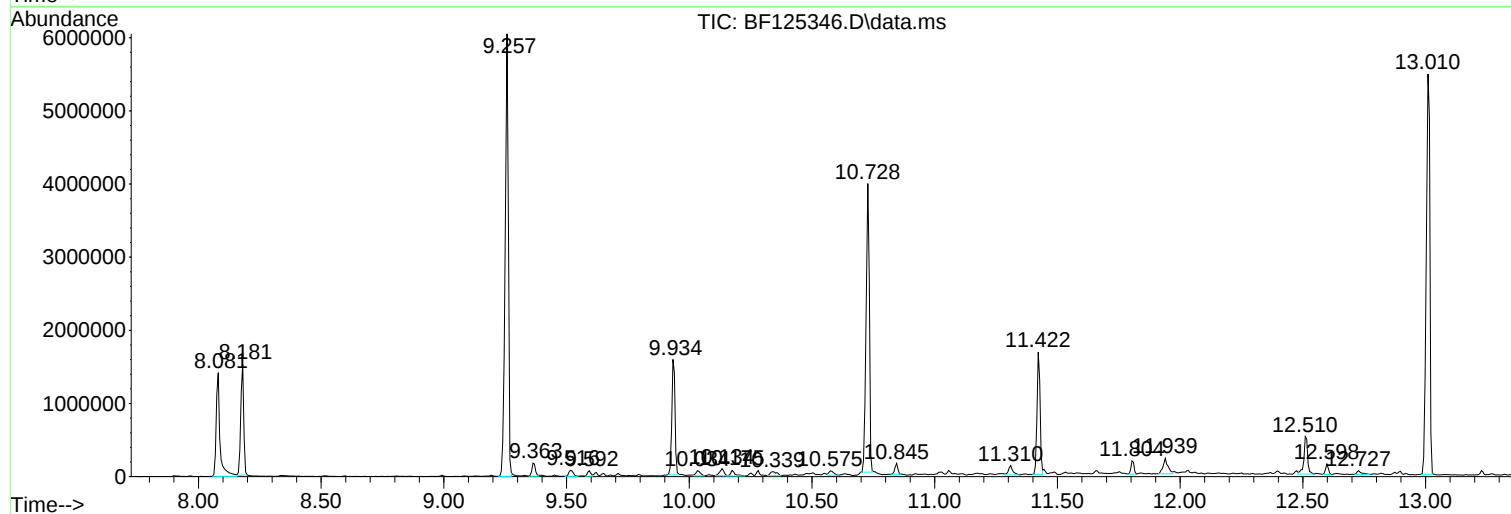
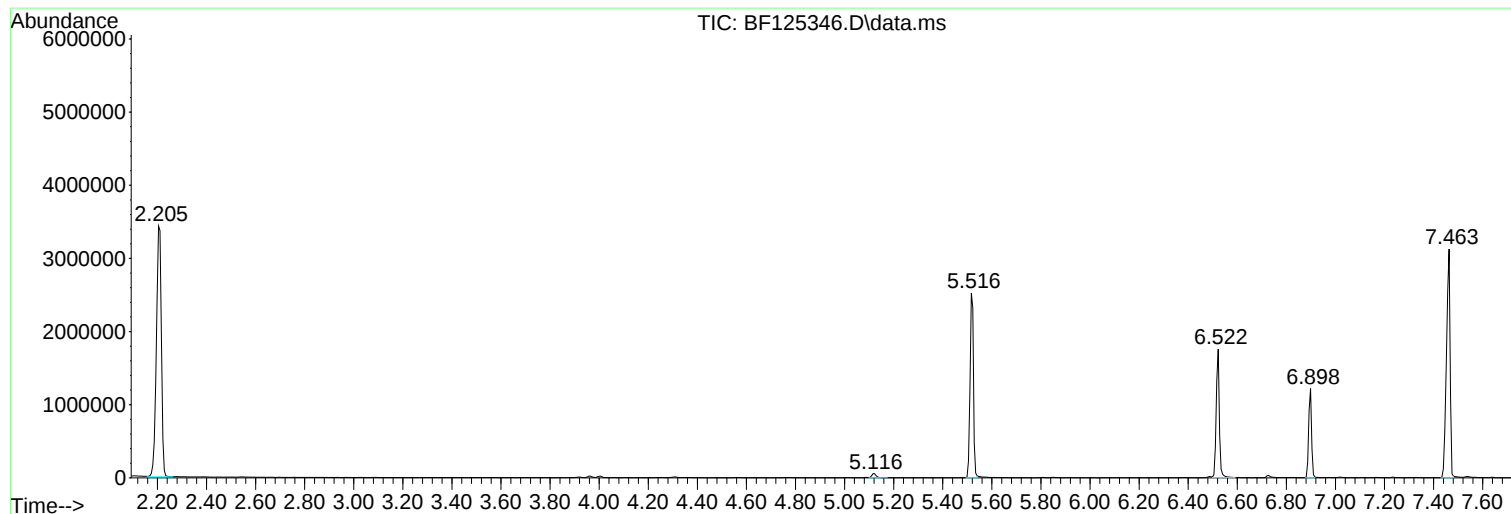
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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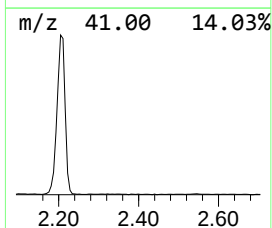
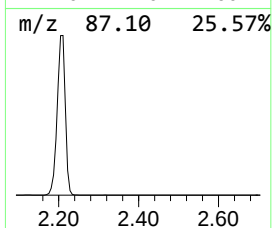
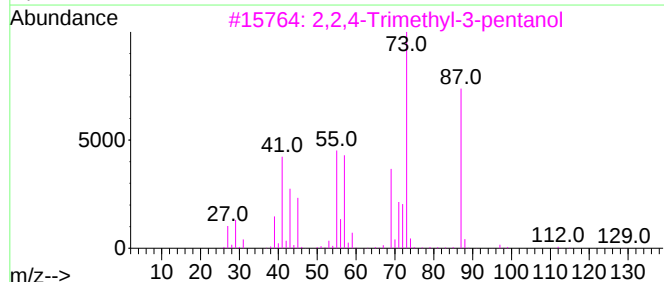
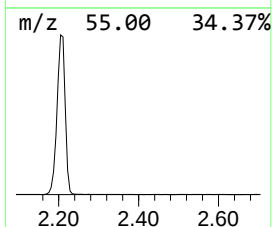
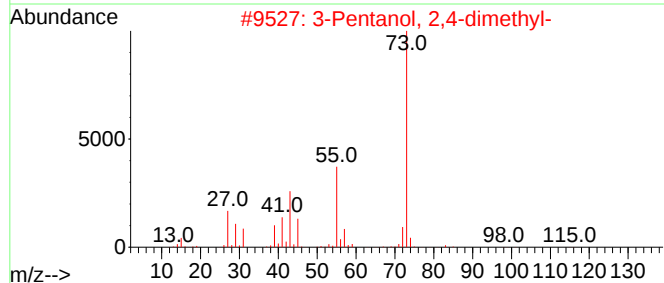
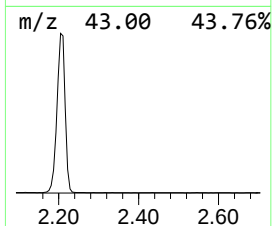
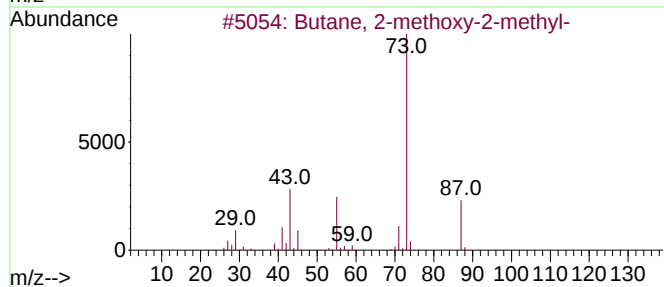
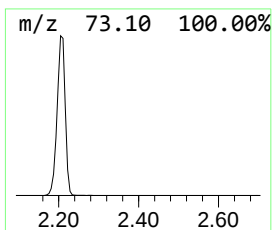
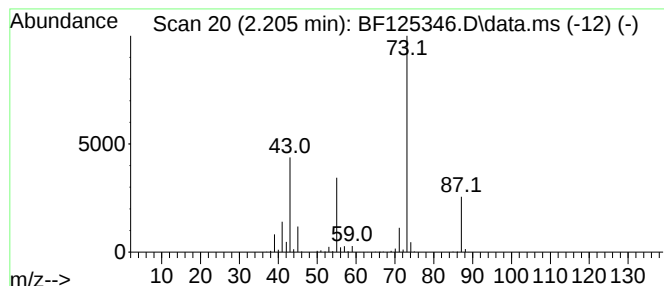
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	98.04 ng	4839460	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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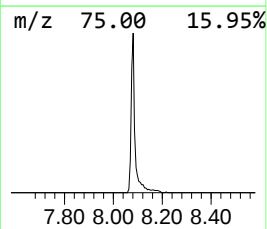
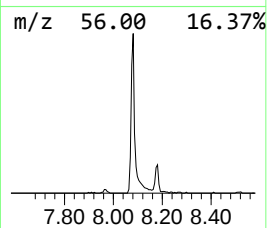
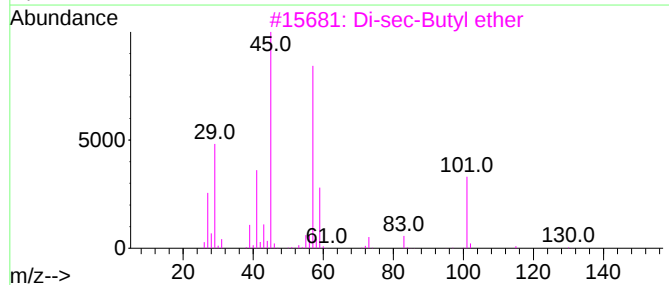
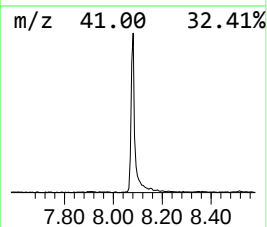
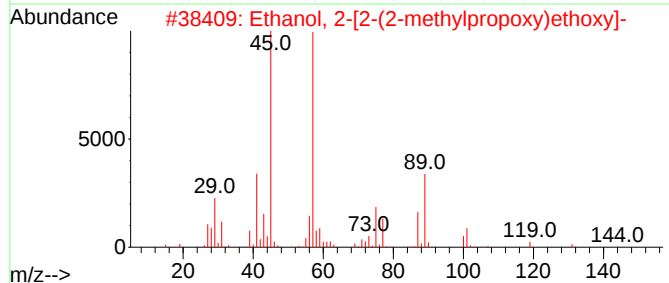
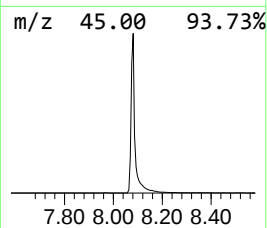
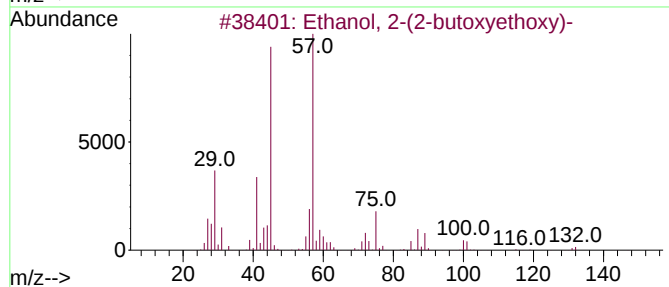
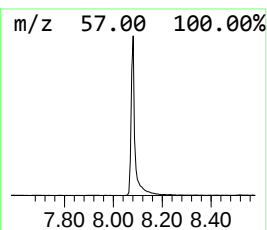
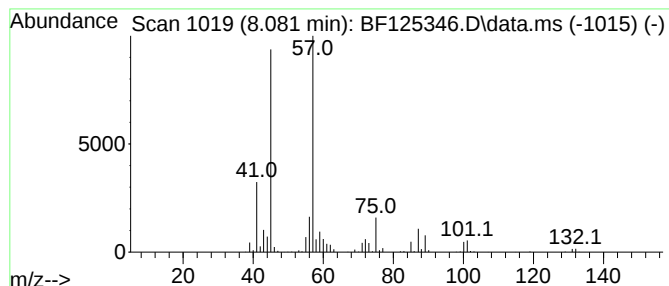
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	23.74 ng	1510810	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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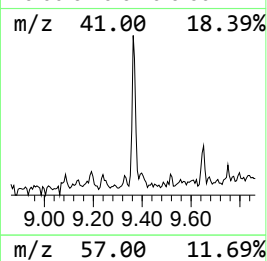
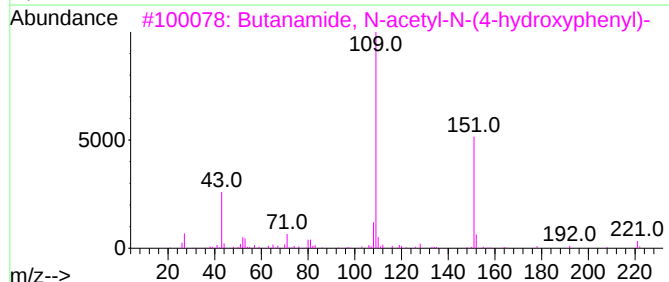
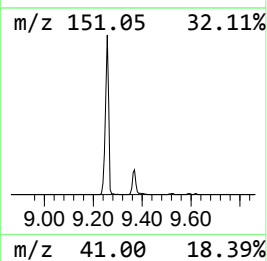
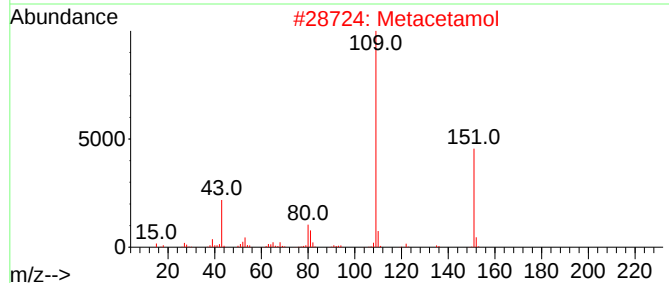
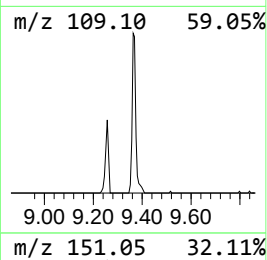
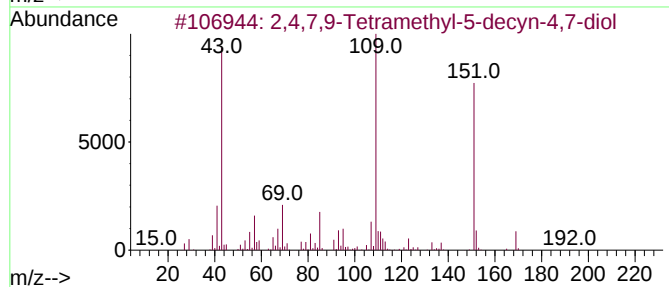
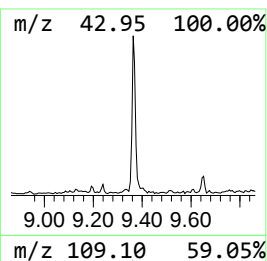
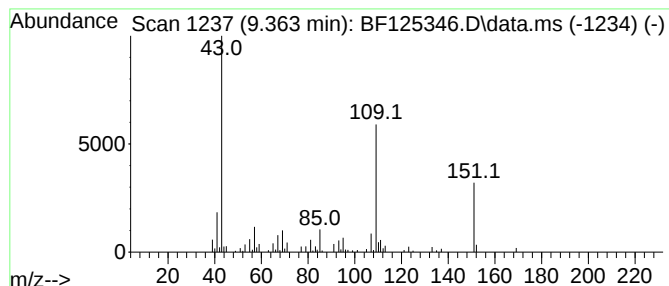
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.363	2.53 ng	179974	Acenaphthene-d10			9.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	86
2	Metacetamol	151	C8H9NO2		000621-42-1	47
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	47
4	benzenamine, 3-[(tetrahydro-2H-p...	193	C11H15NO2		1010400-28-1	38
5	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	38



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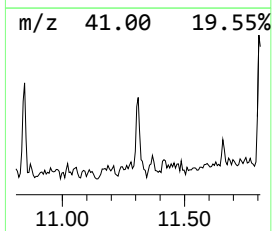
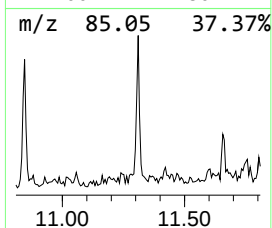
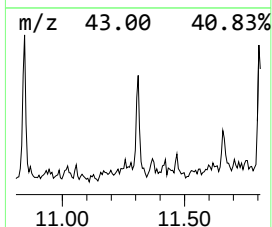
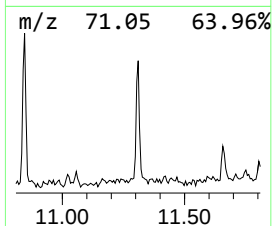
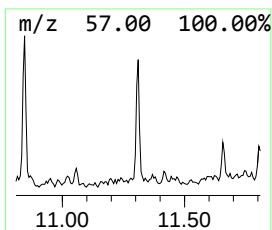
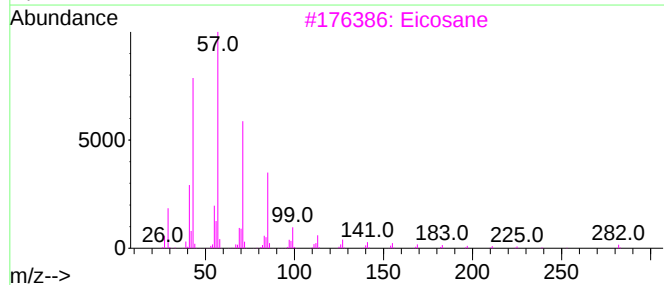
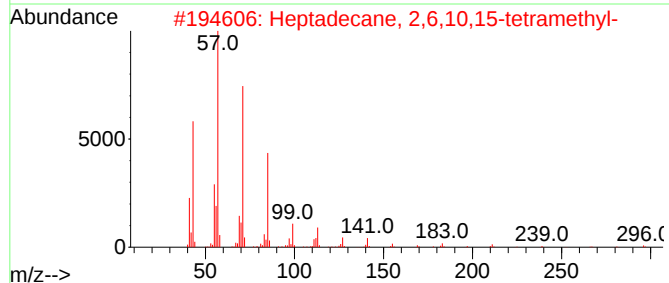
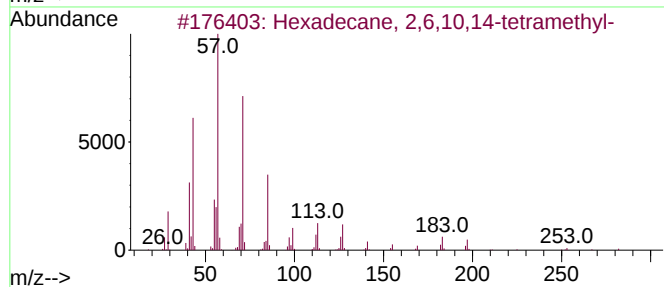
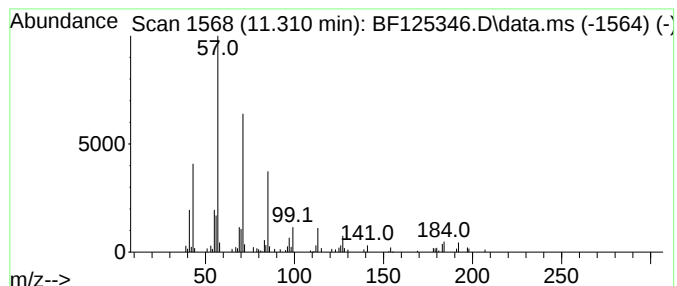
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexadecane, 2,6,10,14-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.310	2.10 ng	153441	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptacosane	380	C27H56	000593-49-7	72
5	Tridecane	184	C13H28	000629-50-5	72



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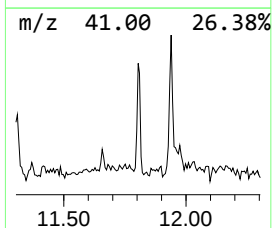
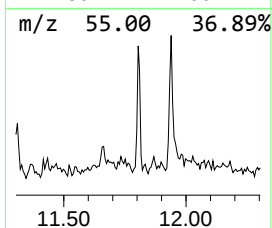
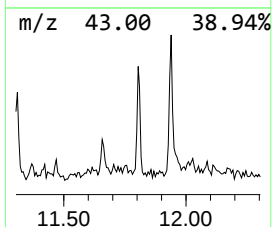
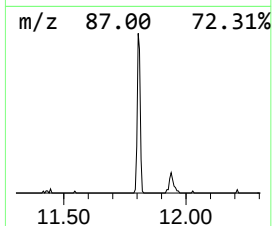
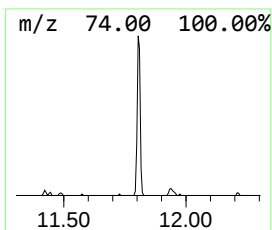
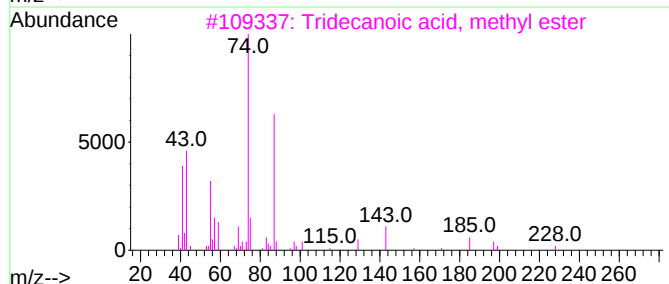
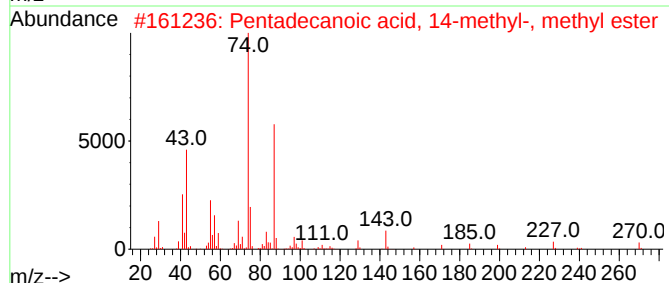
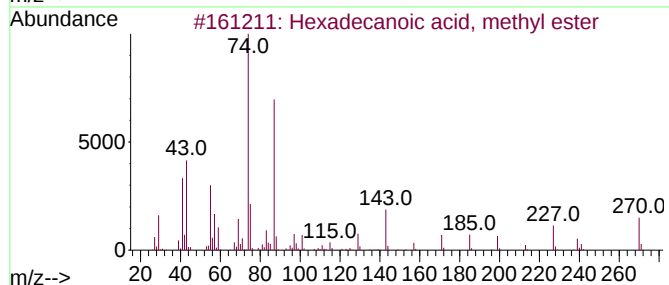
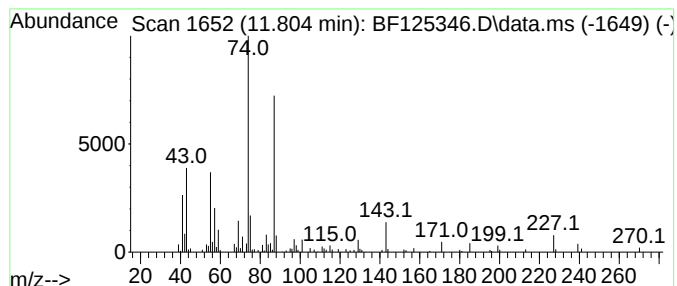
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.12 ng	154639	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125346.D
Acq On : 3 Sep 2021 14:58
Operator : JU/CG
Sample : M3606-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-BFD

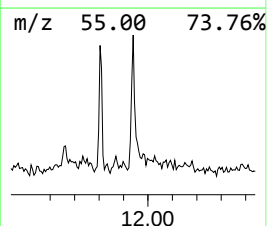
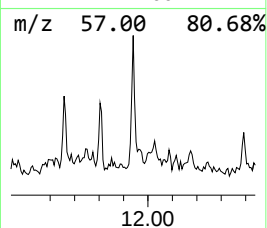
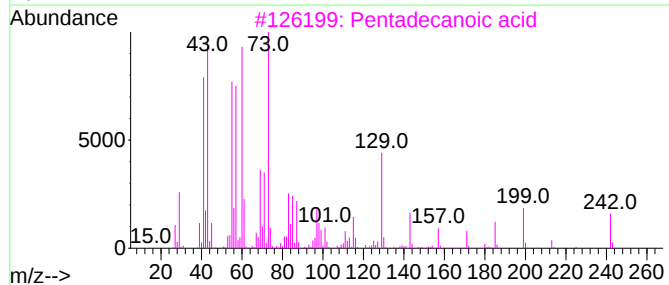
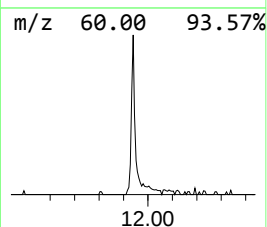
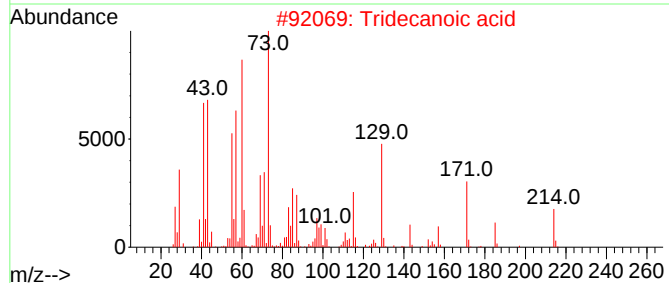
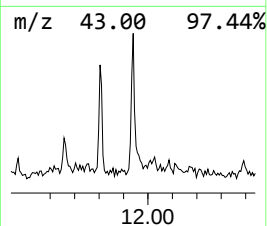
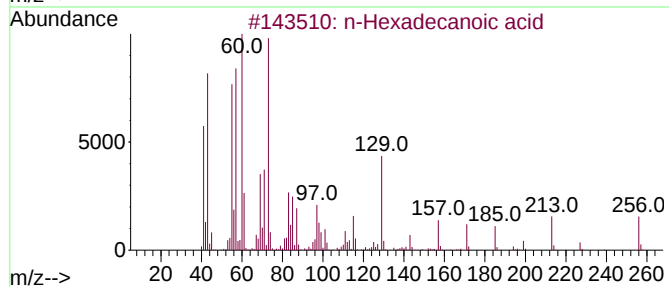
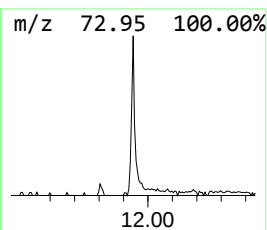
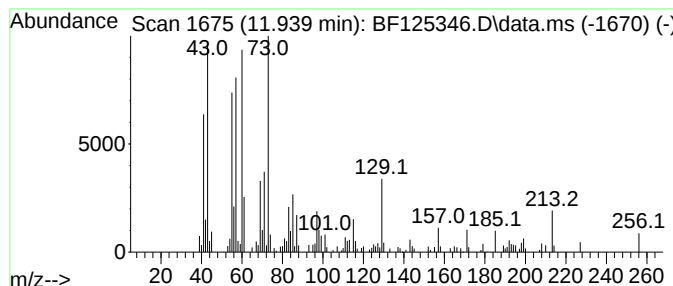
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	4.02 ng	293171	Phenanthrene-d10	11.422

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	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125346.D
Acq On : 3 Sep 2021 14:58
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Sample : M3606-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
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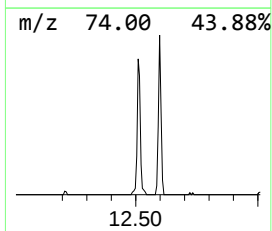
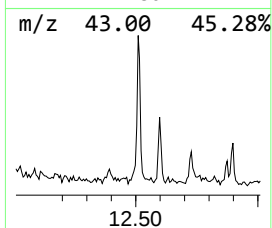
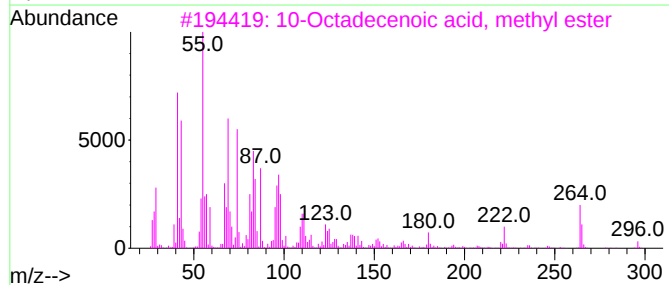
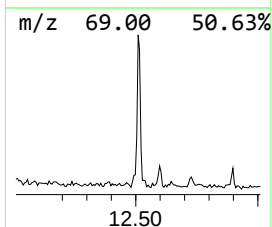
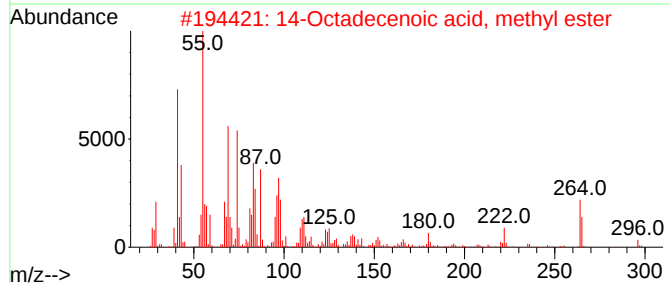
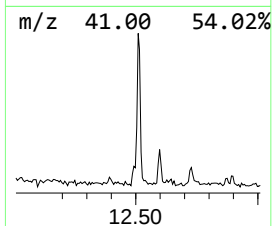
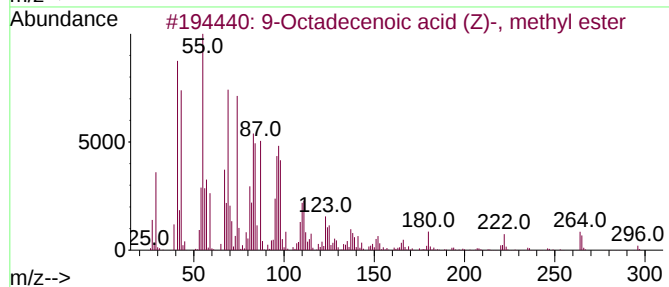
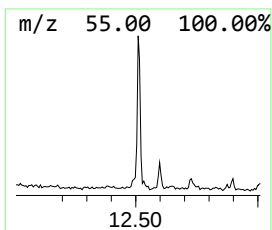
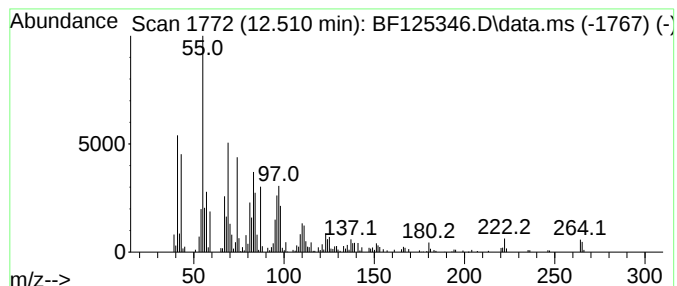
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	7.32 ng	533423	Phenanthrene-d10	11.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
5		(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125346.D
Acq On : 3 Sep 2021 14:58
Operator : JU/CG
Sample : M3606-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-BFD

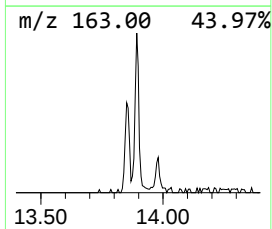
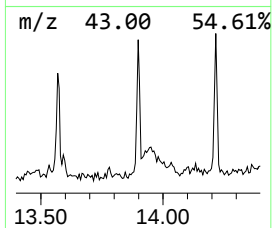
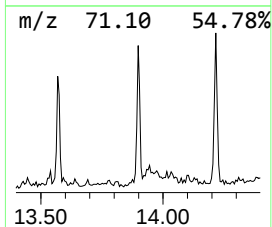
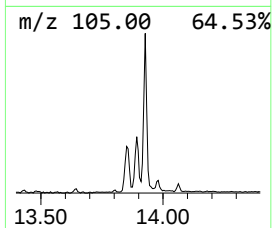
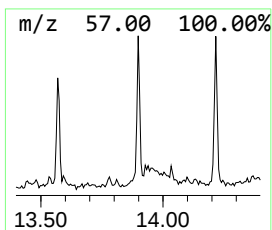
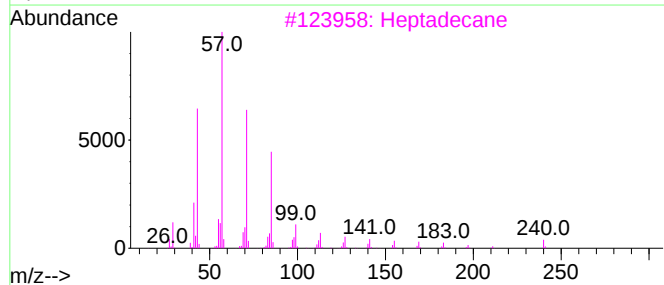
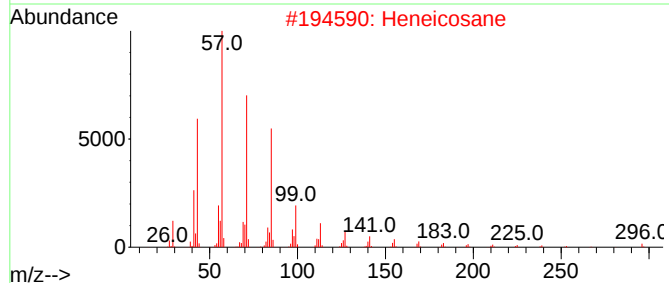
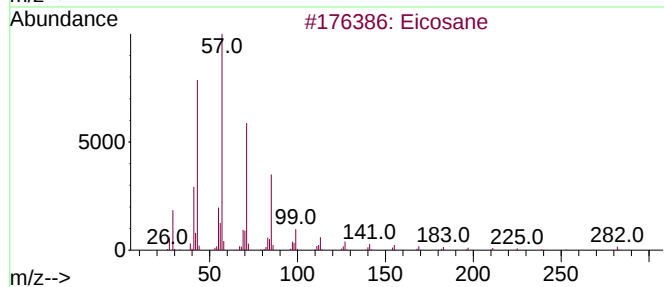
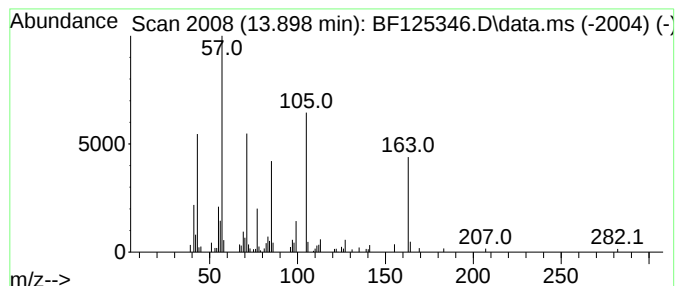
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.76 ng	148667	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heneicosane	296	C21H44	000629-94-7	49
3			Heptadecane	240	C17H36	000629-78-7	49
4			Hexadecane	226	C16H34	000544-76-3	49
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125346.D
Acq On : 3 Sep 2021 14:58
Operator : JU/CG
Sample : M3606-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-BFD

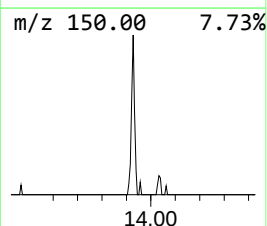
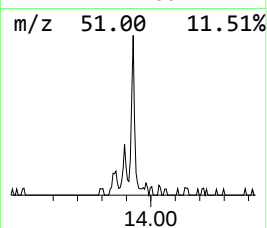
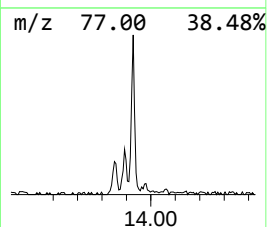
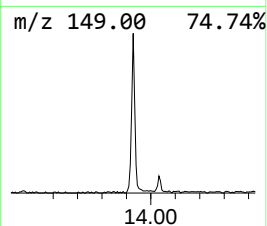
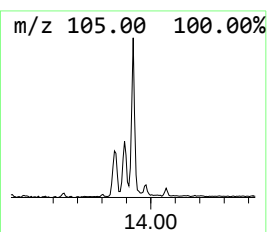
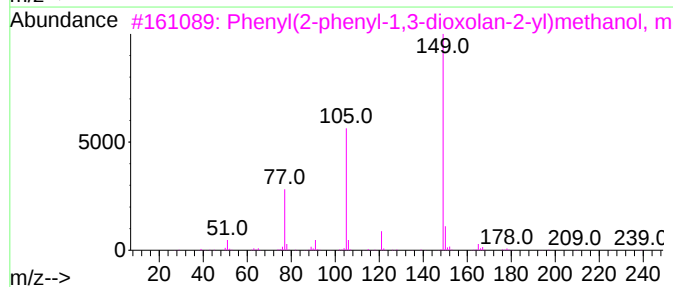
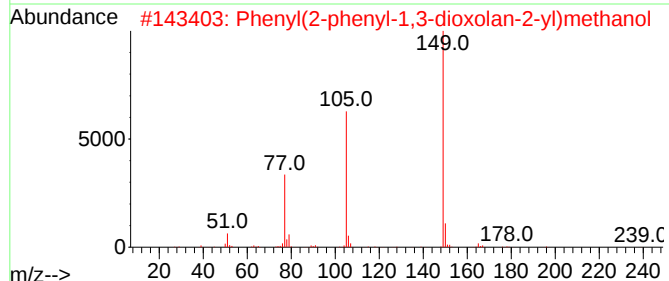
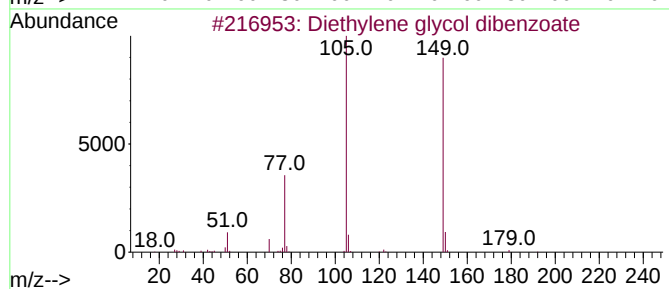
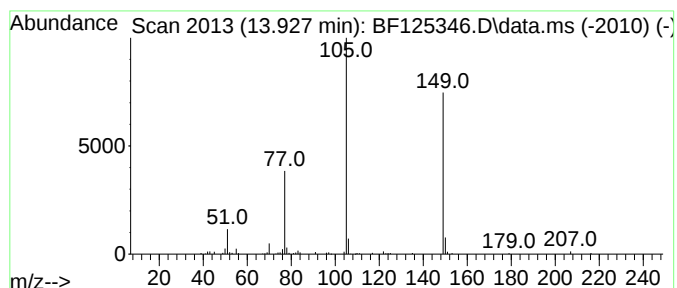
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	3.37 ng	181539	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125346.D
Acq On : 3 Sep 2021 14:58
Operator : JU/CG
Sample : M3606-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BPU-BFD

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	8.081	23.7	ng	1510810	2	8.181	1273060	20.0
2,4,7,9-Tetrame...	9.363	2.5	ng	179974	3	9.934	1421120	20.0
Hexadecane, 2,6...	11.310	2.1	ng	153441	4	11.422	1458390	20.0
Hexadecanoic ac...	11.804	2.1	ng	154639	4	11.422	1458390	20.0
n-Hexadecanoic ...	11.939	4.0	ng	293171	4	11.422	1458390	20.0
9-Octadecenoic ...	12.510	7.3	ng	533423	4	11.422	1458390	20.0
Eicosane	13.898	2.8	ng	148667	5	14.063	1078740	20.0
Diethylene glyc...	13.927	3.4	ng	181539	5	14.063	1078740	20.0