

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
 Data File : BF139579.D
 Acq On : 30 Sep 2024 15:28
 Operator : RC/JU
 Sample : P4192-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-222

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	17	22	29	rBV	13063	20382	1.64%	0.209%
2	3.322	204	209	233	rBV	22676	67178	5.42%	0.689%
3	5.069	496	506	516	rVB	43463	65838	5.31%	0.675%
4	5.481	570	576	581	rBV	848547	1101779	88.88%	11.293%
5	6.493	742	748	753	rBV	925804	1160124	93.59%	11.891%
6	6.692	777	782	794	rVB	17980	26567	2.14%	0.272%
7	6.863	807	811	816	rBV	296411	362279	29.22%	3.713%
8	7.428	901	907	912	rBV	570829	736914	59.45%	7.554%
9	7.675	943	949	955	rBV	12495	17073	1.38%	0.175%
10	8.145	1024	1029	1034	rBV	375707	448758	36.20%	4.600%
11	8.457	1077	1082	1093	rBV	37263	53949	4.35%	0.553%
12	9.216	1206	1211	1216	rBV	1030857	1239626	100.00%	12.706%
13	9.898	1322	1327	1331	rBV	364994	453784	36.61%	4.651%
14	9.986	1337	1342	1350	rBV2	20935	33876	2.73%	0.347%
15	10.098	1355	1361	1365	rBV	18025	23023	1.86%	0.236%
16	10.439	1416	1419	1424	rVB	15459	19475	1.57%	0.200%
17	10.604	1440	1447	1453	rVB	16050	21716	1.75%	0.223%
18	10.680	1455	1460	1475	rVV	350786	439219	35.43%	4.502%
19	11.380	1574	1579	1587	rBV2	327448	491181	39.62%	5.035%
20	11.904	1660	1668	1679	rBV3	56340	125433	10.12%	1.286%
21	11.992	1680	1683	1691	rVB3	11257	21012	1.70%	0.215%
22	12.592	1780	1785	1790	rBV	58623	79393	6.40%	0.814%
23	12.686	1796	1801	1817	rBV	174727	361311	29.15%	3.704%
24	12.816	1819	1823	1829	rVB	43384	68452	5.52%	0.702%
25	12.963	1842	1848	1853	rVB	701654	892312	71.98%	9.146%
26	13.863	1997	2001	2013	rBV3	29732	69726	5.62%	0.715%
27	14.016	2020	2027	2036	rVB	274777	419336	33.83%	4.298%
28	14.174	2051	2054	2058	rBV	12683	17029	1.37%	0.175%
29	14.639	2129	2133	2137	rBV2	38043	65507	5.28%	0.671%
30	14.933	2178	2183	2193	rVB3	99800	185925	15.00%	1.906%
31	15.121	2211	2215	2218	rBV	37039	50244	4.05%	0.515%
32	15.168	2219	2223	2238	rVB5	44075	136324	11.00%	1.397%
33	15.480	2270	2276	2286	rVB	184230	315382	25.44%	3.233%
34	15.704	2311	2314	2328	rVB4	34137	69656	5.62%	0.714%
35	15.933	2348	2353	2361	rBV	51995	96127	7.75%	0.985%

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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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

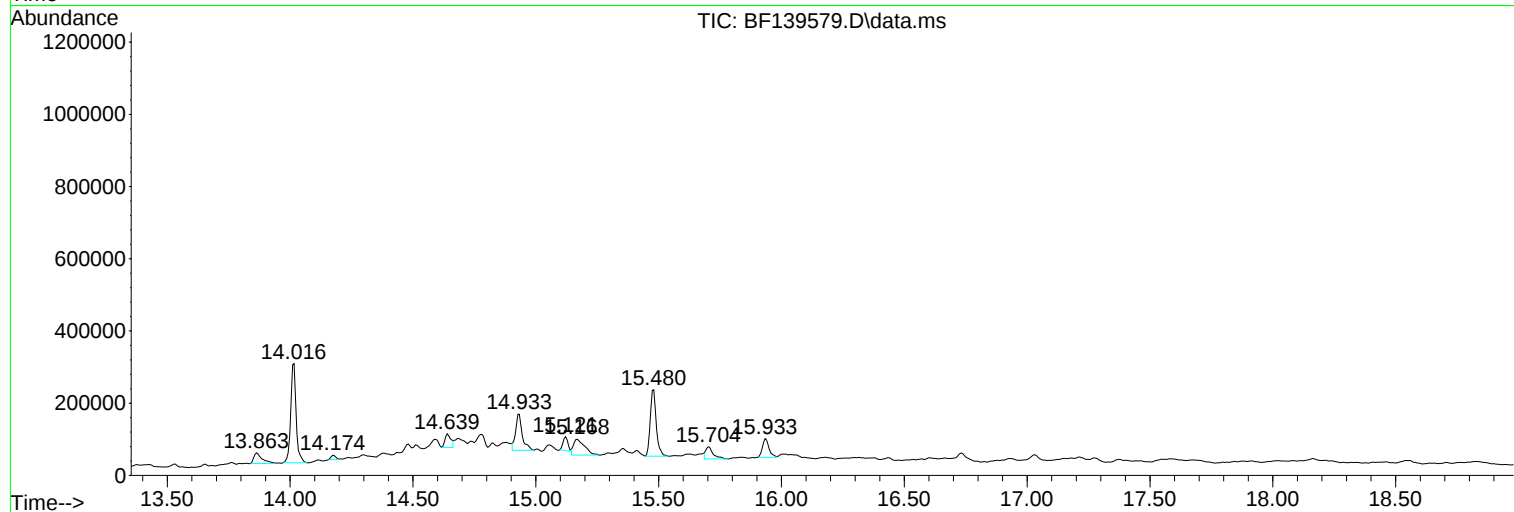
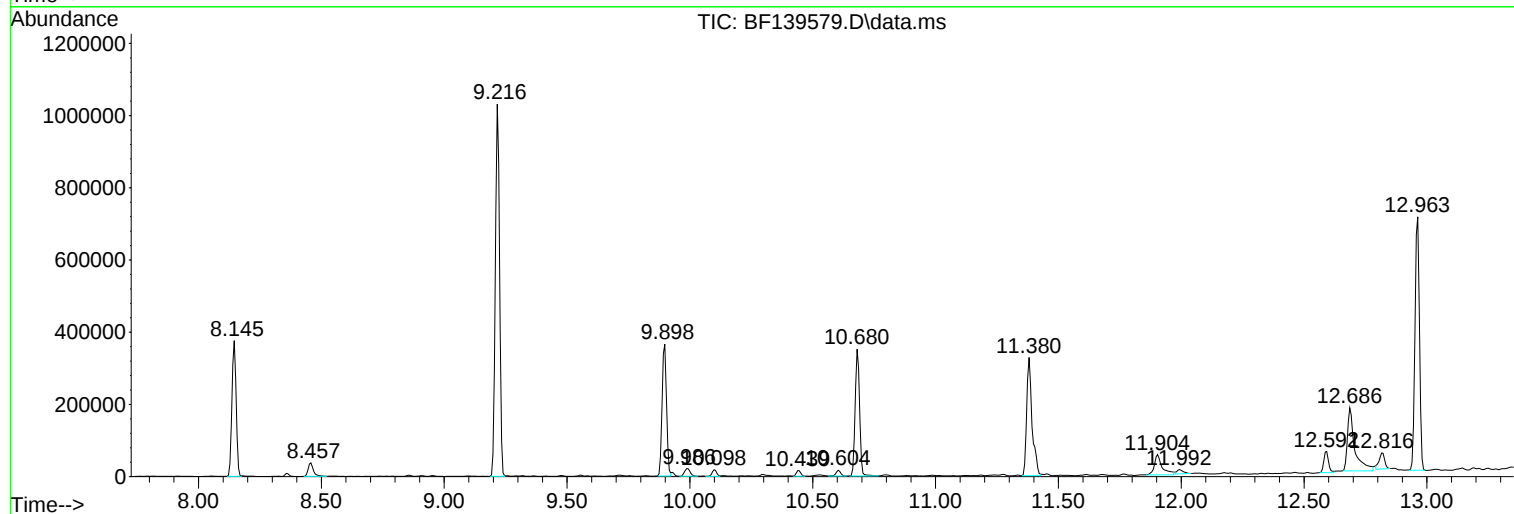
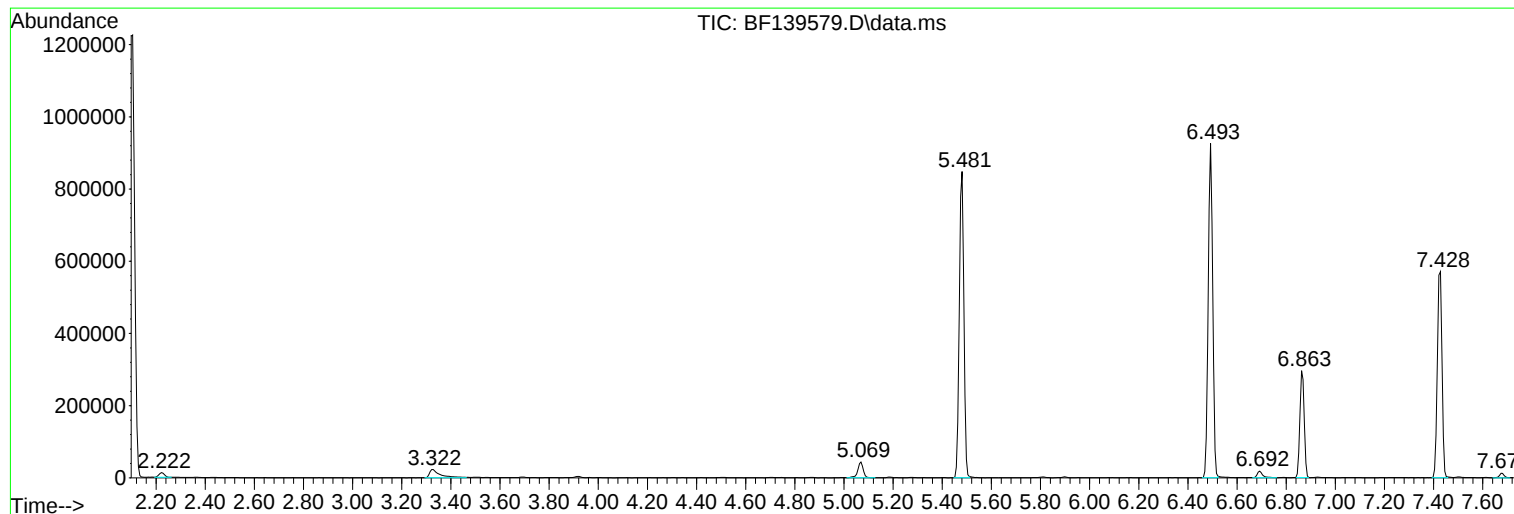
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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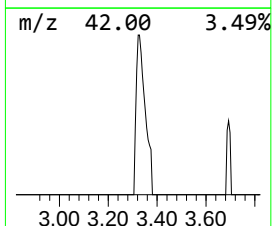
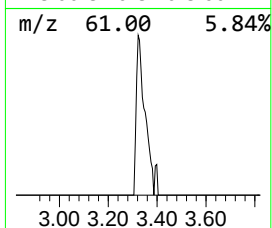
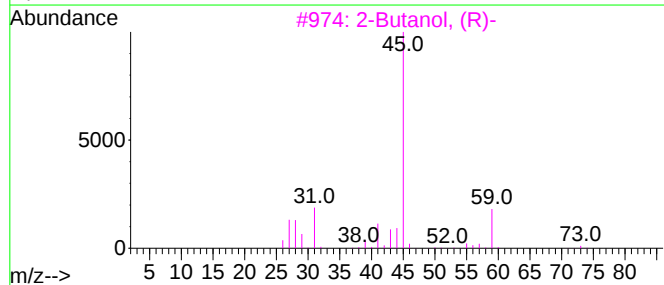
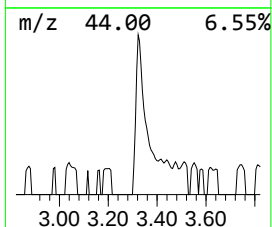
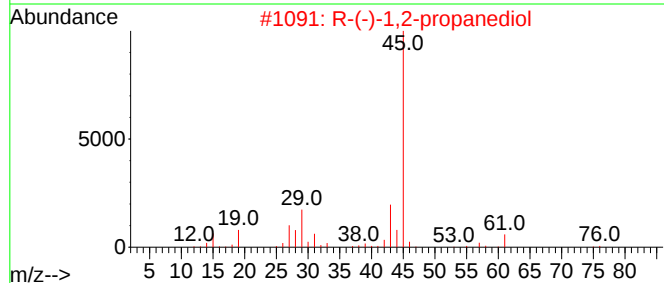
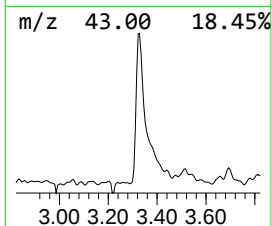
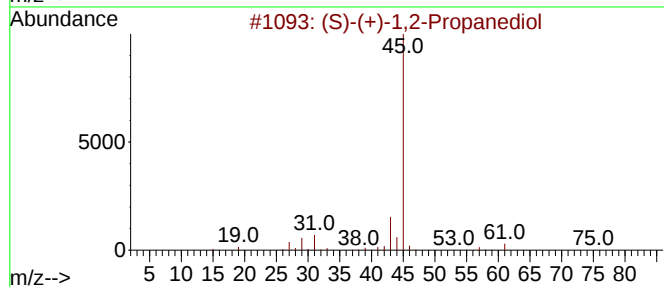
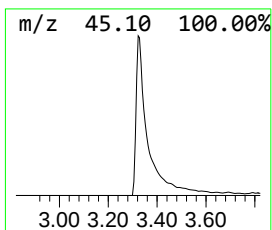
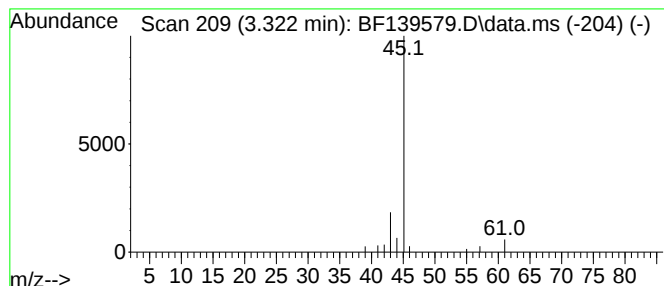
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.322	3.71 ng	67178	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	64
3	2-Butanol, (R)-			74	C4H10O	014898-79-4	9
4	2,3-Butanediol			90	C4H10O2	000513-85-9	9
5	Propylene Glycol			76	C3H8O2	000057-55-6	9



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Misc :
ALS Vial : 11 Sample Multiplier: 1

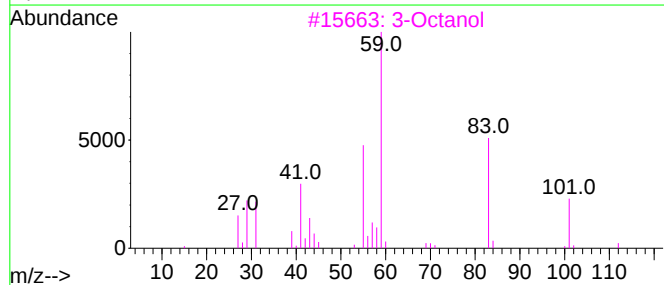
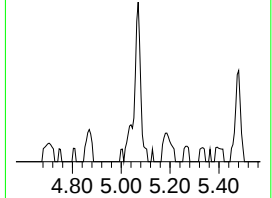
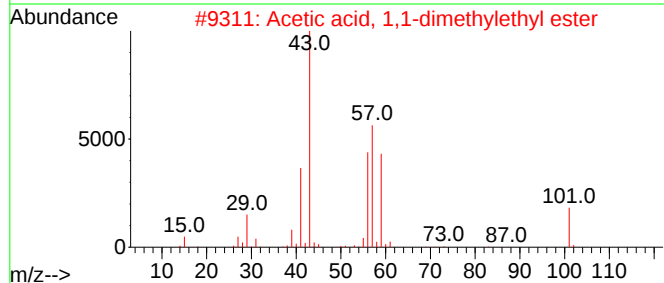
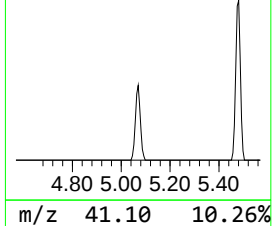
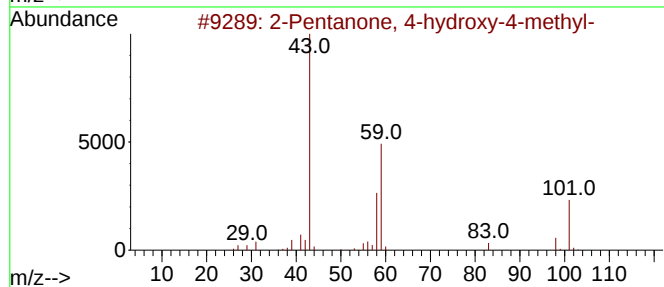
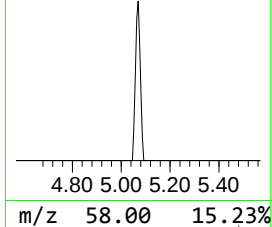
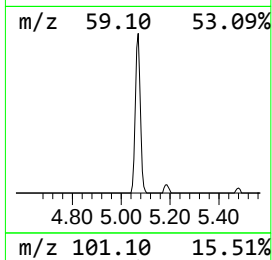
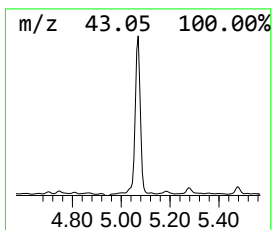
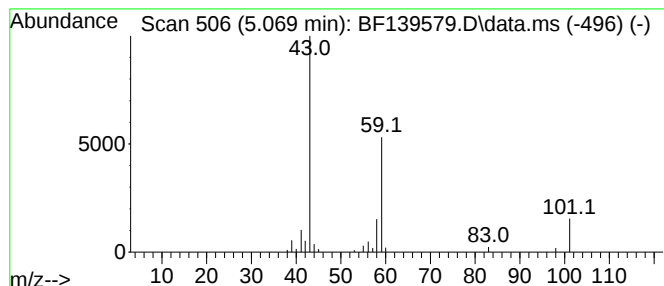
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.069	3.63 ng	65838	1,4-Dichlorobenzene-d4		6.863	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	39
3	3-Octanol		130	C8H18O	000589-98-0	36
4	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	16



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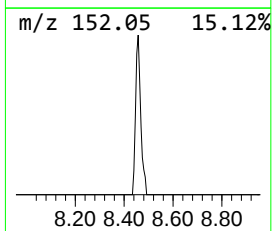
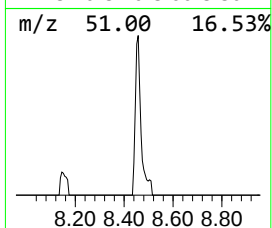
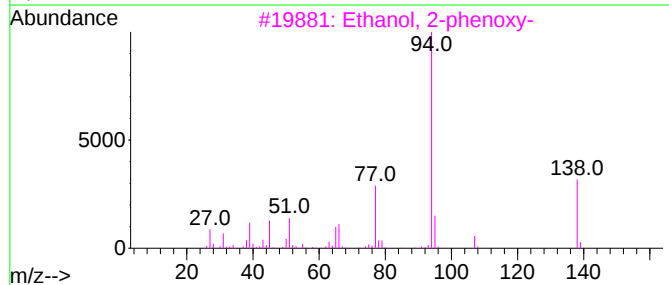
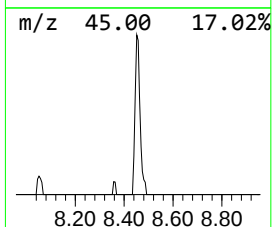
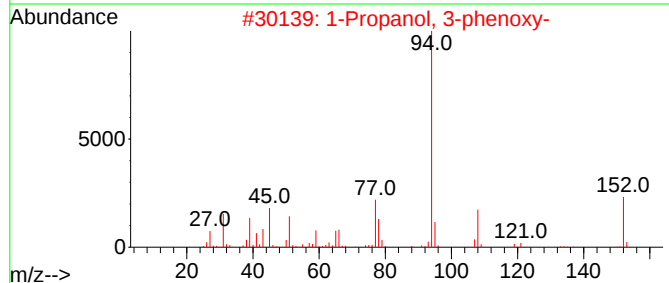
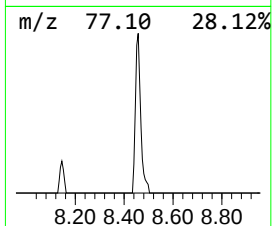
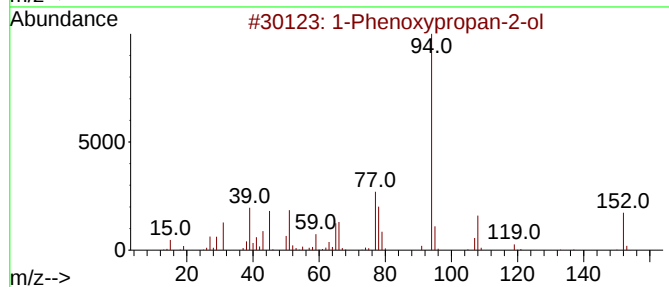
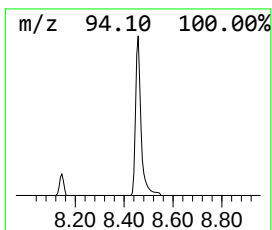
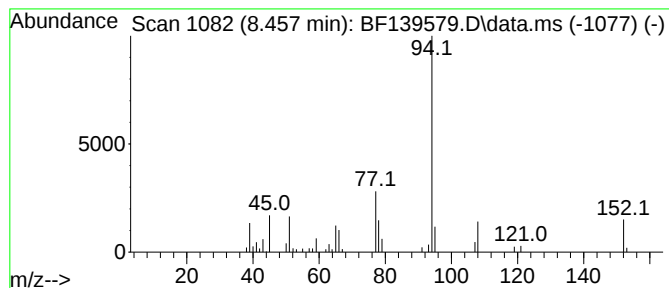
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.40 ng	53949	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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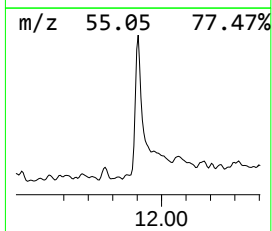
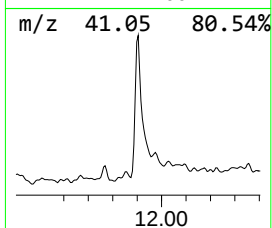
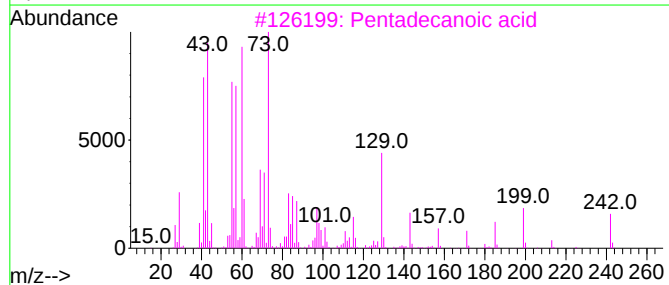
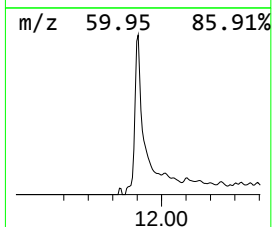
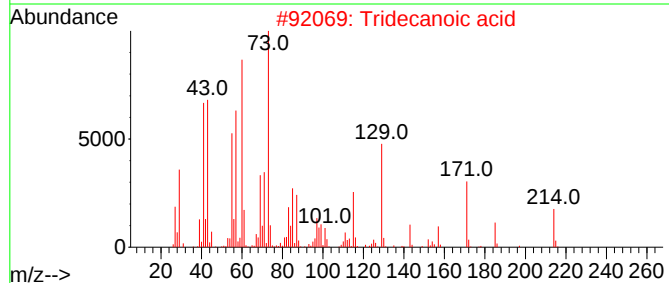
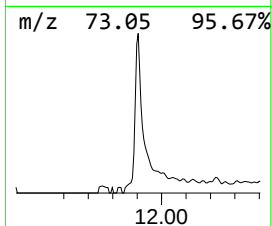
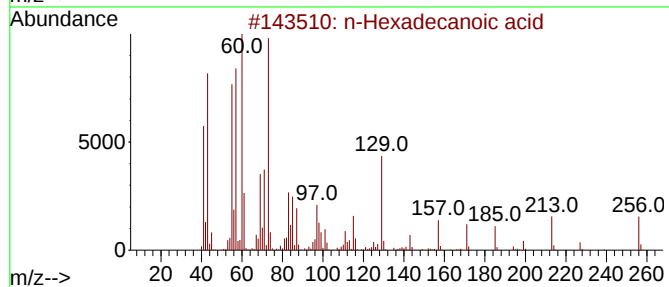
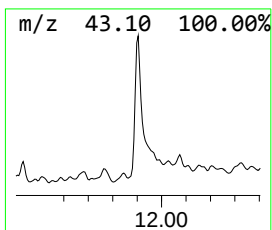
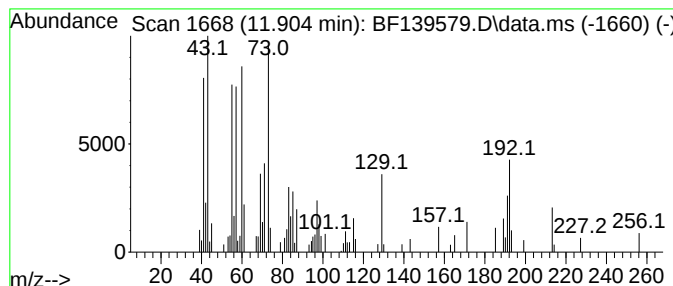
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	5.11 ng	125433	Phenanthrene-d10	11.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		n-Butyl n-pentyl disulfide	192	C9H20S2	072437-52-6	18



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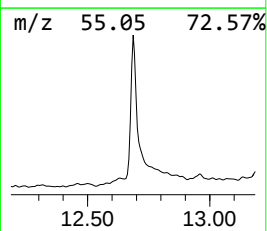
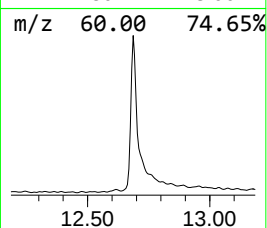
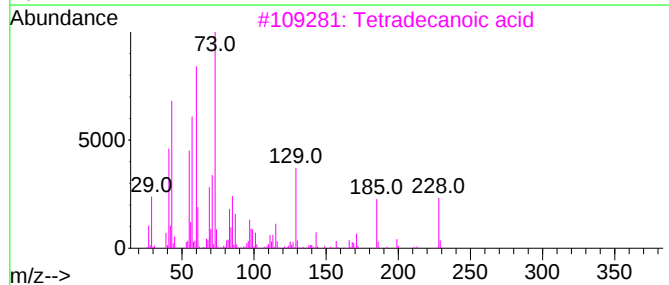
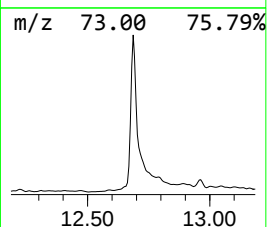
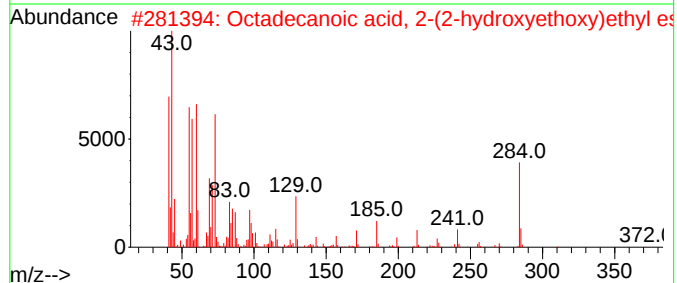
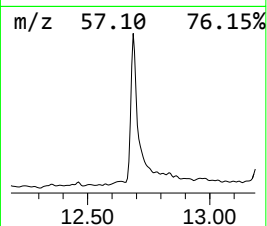
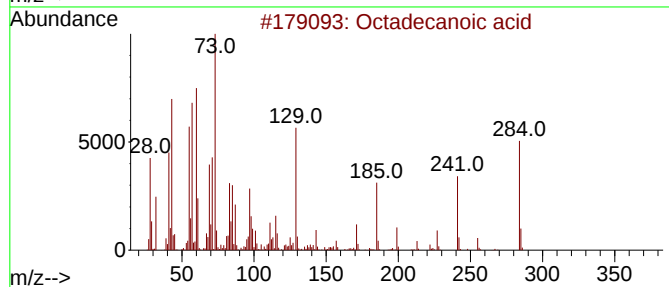
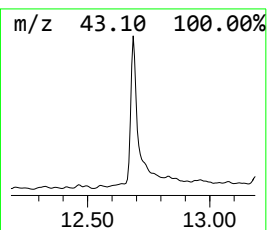
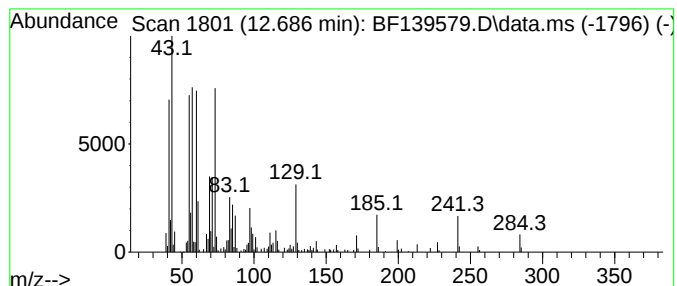
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	14.71 ng	361311	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
Operator : RC/JU
Sample : P4192-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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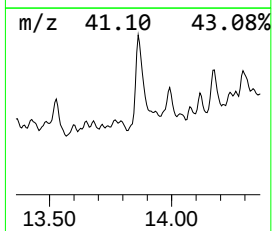
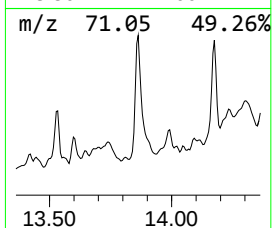
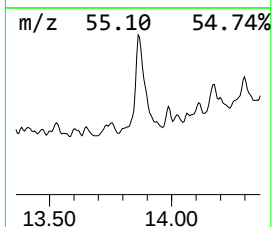
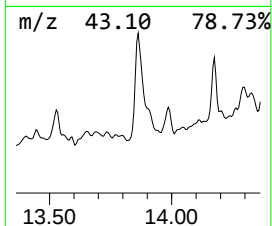
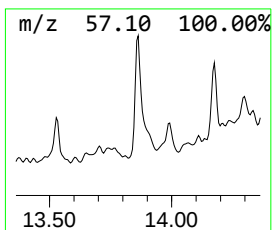
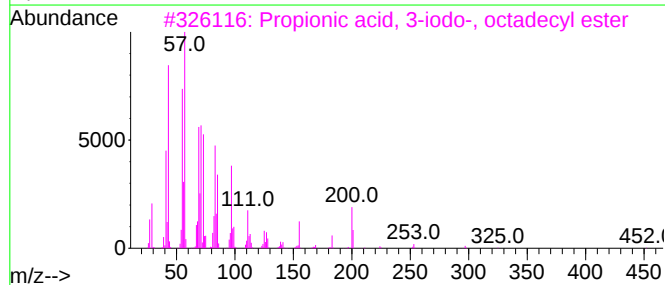
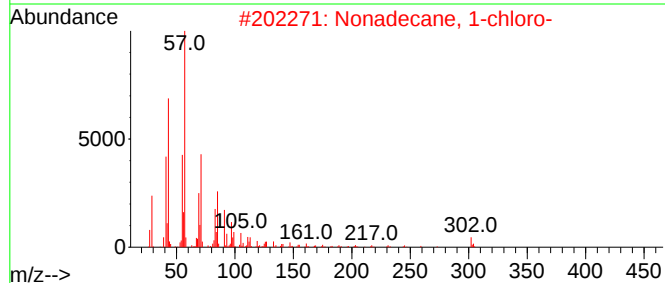
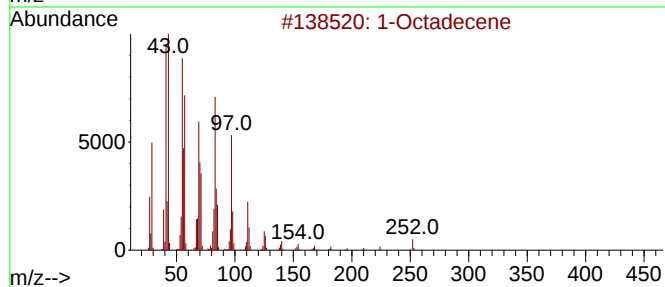
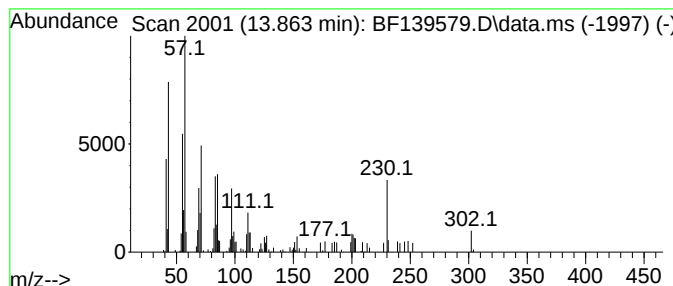
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.33 ng	69726	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	70
2	Nonadecane, 1-chloro-			302	C19H39Cl	062016-76-6	64
3	Propionic acid, 3-iodo-, octadec...			452	C21H41IO2	1000406-24-9	64
4	Sulfurous acid, octadecyl 2-prop...			376	C21H44O3S	1000309-12-7	62
5	Oxalic acid, isobutyl tetradecyl...			342	C20H38O4	1000309-37-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
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Sample : P4192-01
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ClientSampleId :
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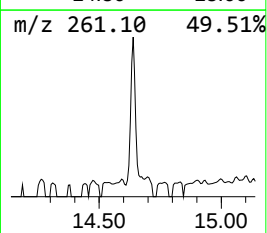
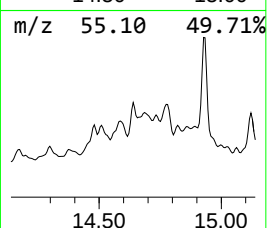
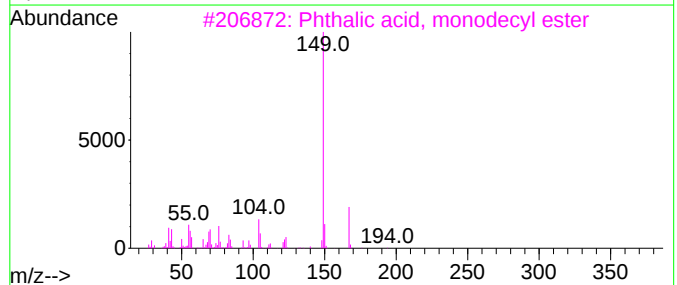
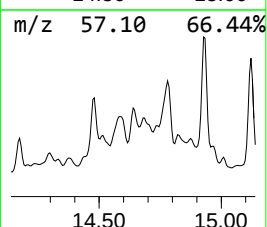
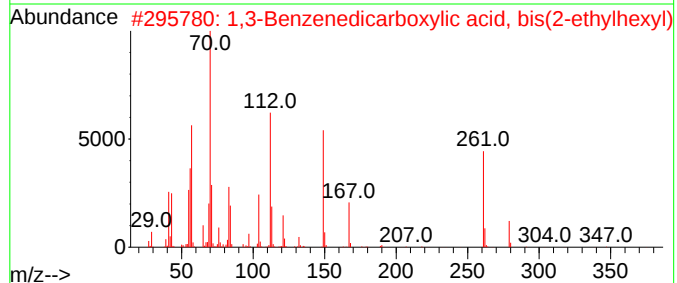
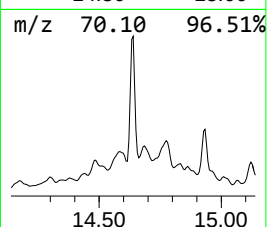
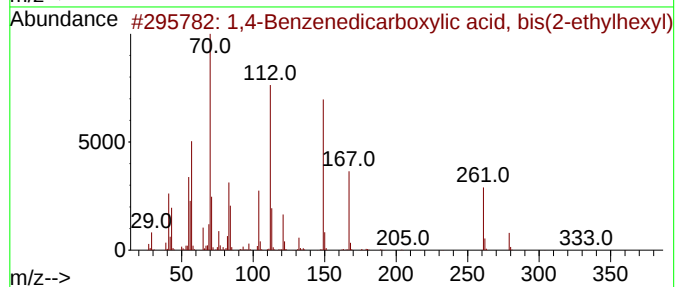
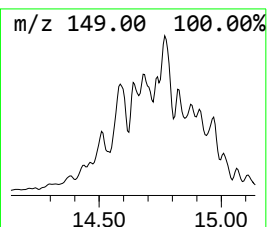
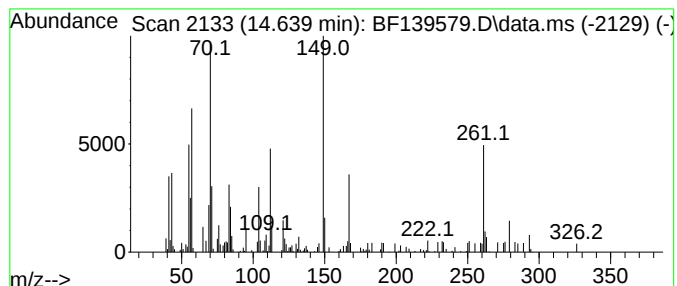
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	3.12 ng	65507	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
3			Phthalic acid, monodecyl ester	306	C18H26O4	024539-60-4	43
4			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	27
5			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
Operator : RC/JU
Sample : P4192-01
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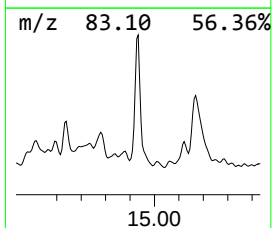
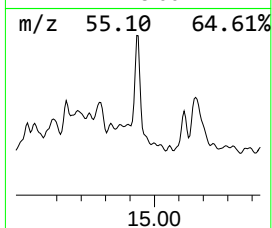
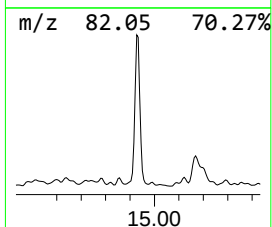
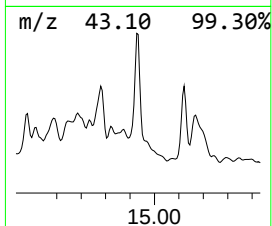
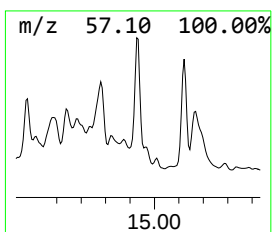
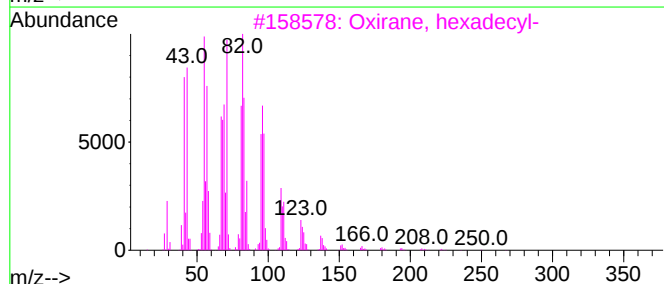
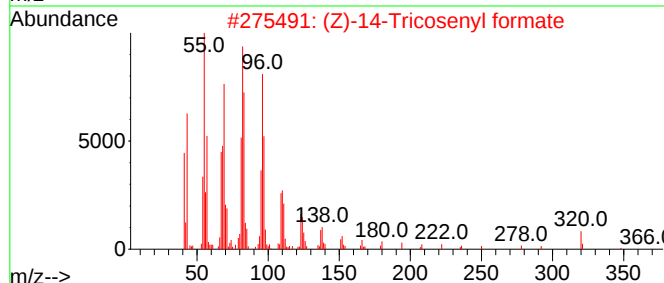
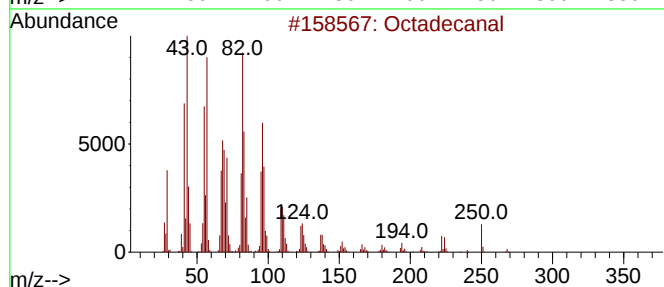
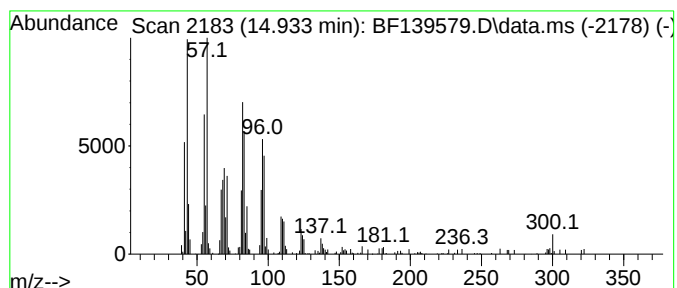
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.933	11.79 ng	185925	Perylene-d12	15.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	93
2	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	86
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80
4	Eicosanal-	296	C20H40O	002400-66-0	76
5	1,19-Eicosadiene	278	C20H38	014811-95-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
Operator : RC/JU
Sample : P4192-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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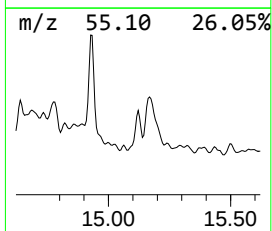
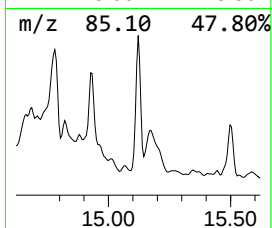
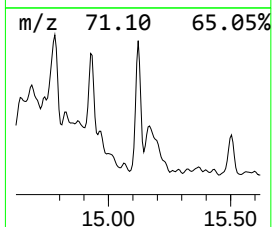
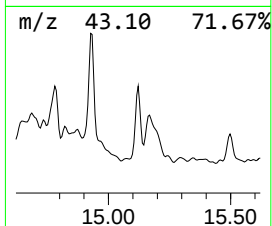
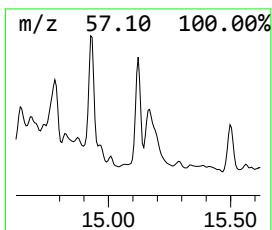
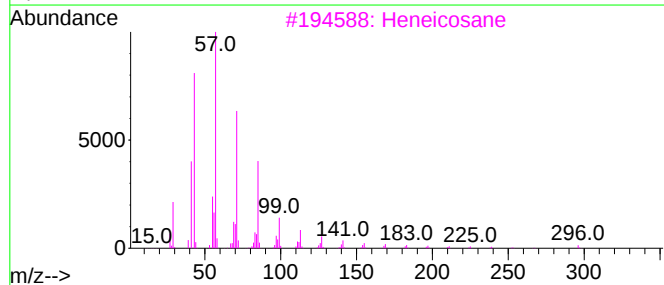
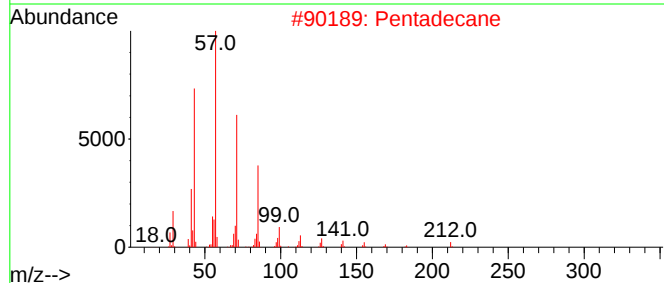
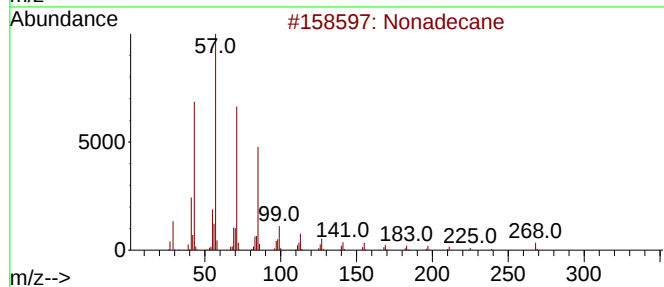
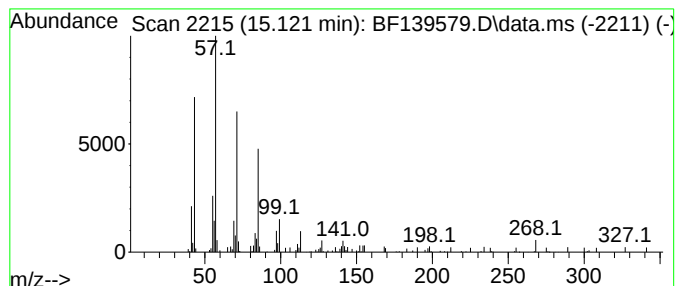
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	3.19 ng	50244	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Pentadecane	212	C15H32	000629-62-9	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
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Sample : P4192-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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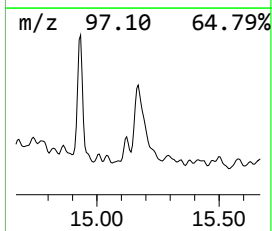
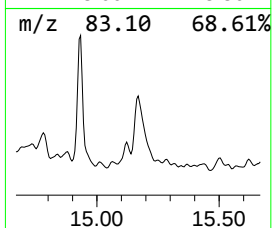
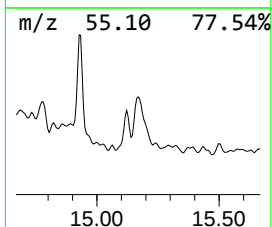
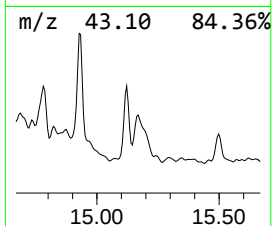
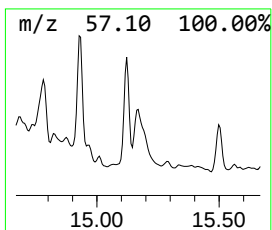
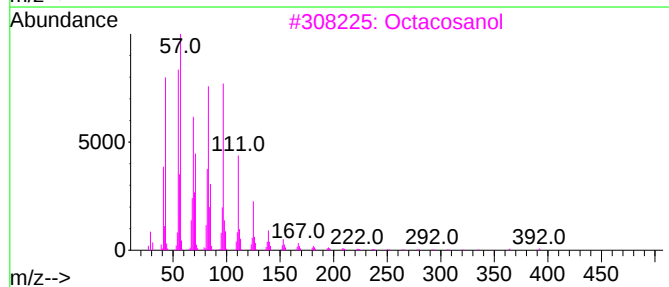
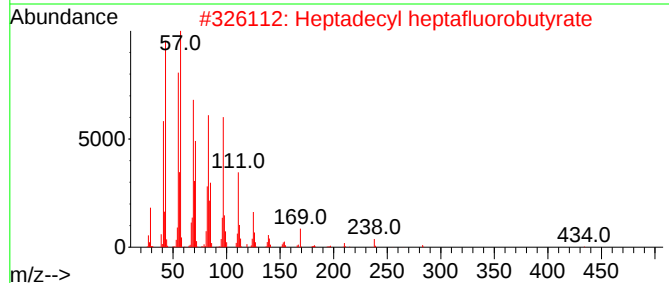
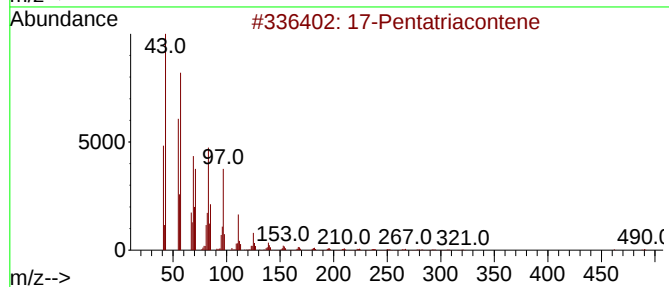
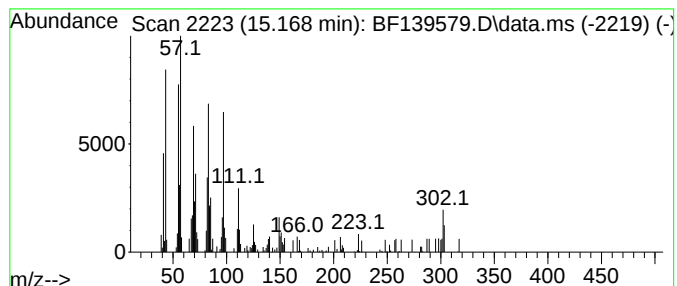
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	8.65 ng	136324	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	76
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
3			Octacosanol	410	C28H58O	000557-61-9	70
4			Octacosyl acetate	452	C30H60O2	018206-97-8	70
5			Behenic alcohol	326	C22H46O	000661-19-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
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Instrument :
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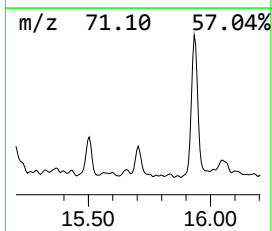
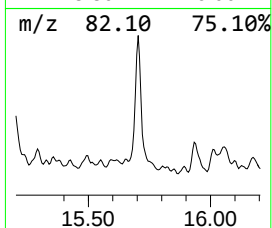
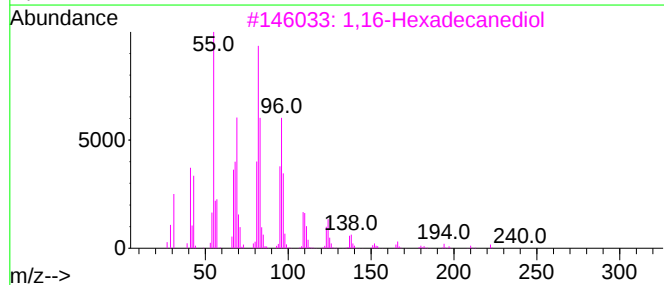
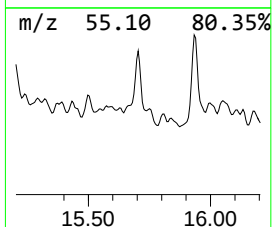
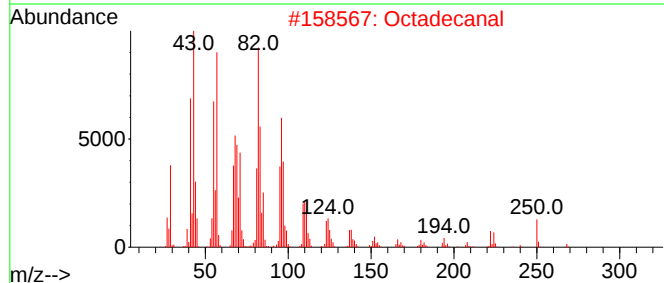
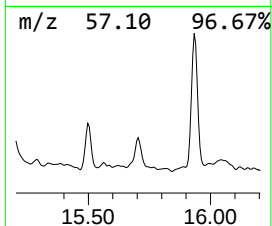
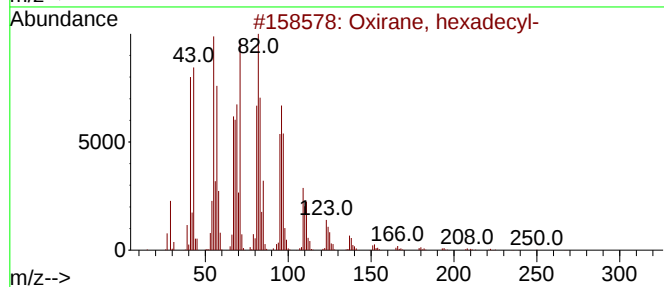
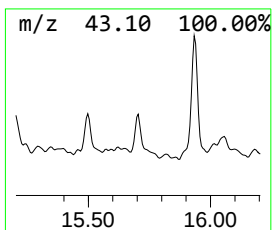
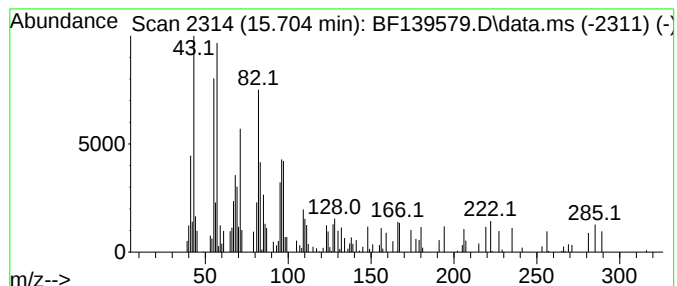
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.704	4.42 ng	69656	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
2			Octadecanal	268	C18H36O	000638-66-4	62
3			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
4			11-Eicosenol	296	C20H40O	1010424-20-3	53
5			E-11-Hexadecen-1-ol	240	C16H32O	1000130-89-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
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ALS Vial : 11 Sample Multiplier: 1

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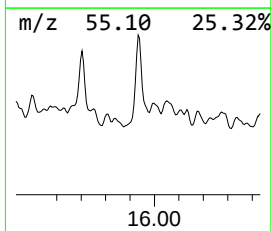
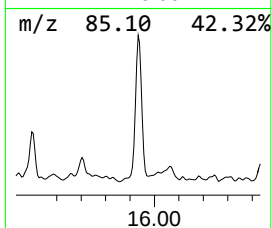
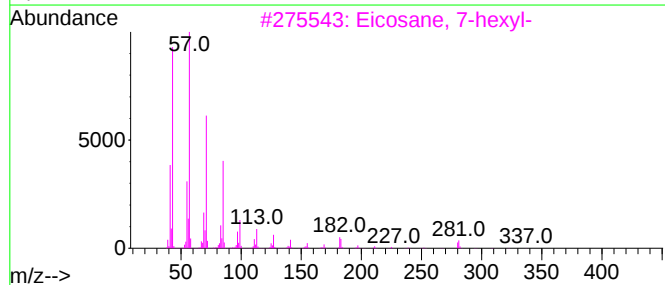
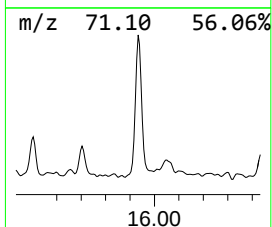
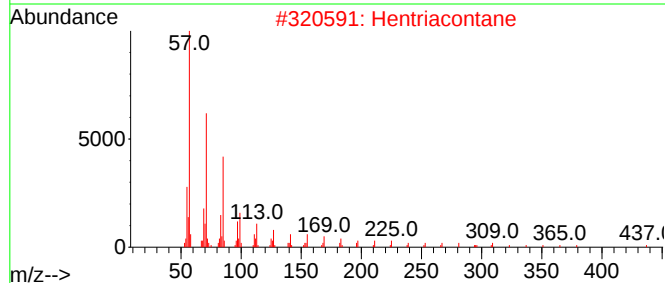
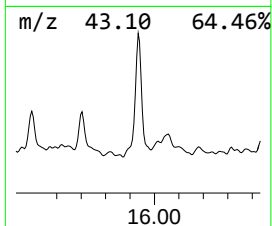
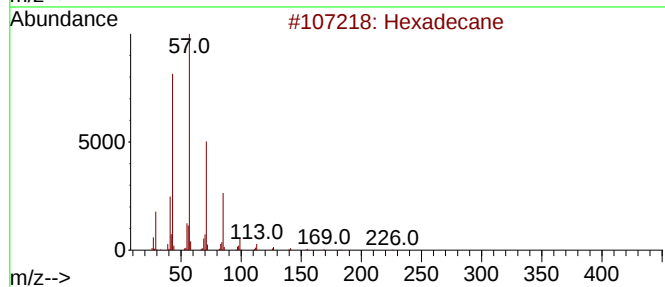
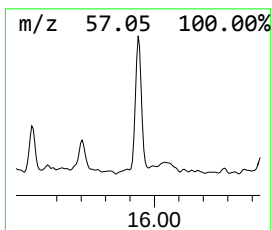
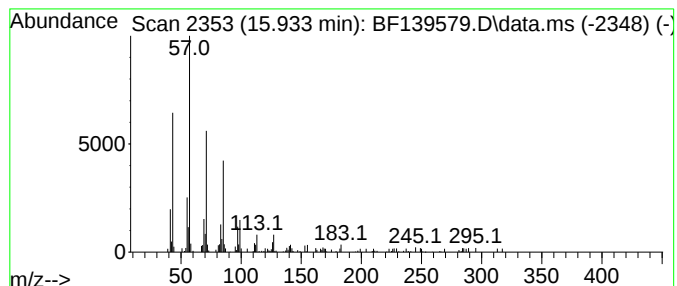
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	6.10 ng	96127	Perylene-d12	15.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	93
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093024\
Data File : BF139579.D
Acq On : 30 Sep 2024 15:28
Operator : RC/JU
Sample : P4192-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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
(S)-(+)-1,2-Pro...	3.322	3.7	ng	67178	1	6.863	362279	20.0
2-Pentanone, 4-...	5.069	3.6	ng	65838	1	6.863	362279	20.0
1-Phenoxypropan...	8.457	2.4	ng	53949	2	8.145	448758	20.0
n-Hexadecanoic ...	11.904	5.1	ng	125433	4	11.380	491181	20.0
Octadecanoic acid	12.686	14.7	ng	361311	4	11.380	491181	20.0
1-Octadecene	13.863	3.3	ng	69726	5	14.015	419336	20.0
1,4-Benzenedica...	14.639	3.1	ng	65507	5	14.015	419336	20.0
Octadecanal	14.933	11.8	ng	185925	6	15.480	315382	20.0
Nonadecane	15.121	3.2	ng	50244	6	15.480	315382	20.0
17-Pentatriacon...	15.168	8.7	ng	136324	6	15.480	315382	20.0
Oxirane, hexade...	15.704	4.4	ng	69656	6	15.480	315382	20.0
Hexadecane	15.933	6.1	ng	96127	6	15.480	315382	20.0