LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125373.D
Acq On : 4 Sep 2021 17:17
Operator : JU/CG
Sample : M3648-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211059-SI-COMP-4-MODIFIED-EL

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: BF125373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	12	20	29	rVB	2660421	3704819	100.00%	14.067%
2	5.116	512	515	522	rBV	56205	63077	1.70%	0.240%
3	5.522	580	584	596	rBV	1847197	1828419	49.35%	6.943%
4	6.522	750	754	766	rBV	1698300	1491558	40.26%	5.664%
5	6.898	814	818	821	rBV	971261	803599	21.69%	3.051%
6	7.457	905	913	917	rBV	2181082	2154841	58.16%	8.182%
7	7.545	924	928	941	rVB6	22830	45831	1.24%	0.174%
8	8.086	1015	1020	1026	rBV2	38448	71438	1.93%	0.271%
9	8.180	1032	1036	1051	rVB	1126651	1024172	27.64%	3.889%
10	9.257	1214	1219	1222	rBV	3757140	3601907	97.22%	13.677%
11	9.933	1326	1334	1343	rBV	1155188	1077757	29.09%	4.092%
12	10.345	1400	1404	1409	rVB4	22734	39586	1.07%	0.150%
13	10.574	1440	1443	1450	rVB3	29019	38995	1.05%	0.148%
14	10.721	1464	1468	1485	rVB	2128145	2166524	58.48%	8.226%
15	10.845	1485	1489	1492	rBV	55945	56992	1.54%	0.216%
16	11.310	1565	1568	1574	rVB4	29622	40841	1.10%	0.155%
17	11.421	1583	1587	1594	rBV	1145299	990403	26.73%	3.761%
18	11.580	1611	1614	1618	rBV	1540226	1168428	31.54%	4.437%
19	11.804	1649	1652	1655	rVB	75143	56355	1.52%	0.214%
20	11.939	1670	1675	1680	rBV4	217373	237268	6.40%	0.901%
21	11.980	1680	1682	1689	rVB	42116	50166	1.35%	0.190%
22	12.727	1805	1809	1816	rBV2	62976	77132	2.08%	0.293%
23	12.868	1830	1833	1836	rVB	43081	41169	1.11%	0.156%
24	13.010	1852	1857	1860	rBV	3280765	3083563	83.23%	11.709%
25	13.927	2009	2013	2029	rVV4	98882	213175	5.75%	0.809%
26	14.062	2033	2036	2044	rVB	887484	764829	20.64%	2.904%
27	14.815	2161	2164	2171	rBV2	113018	154136	4.16%	0.585%
28	15.174	2223	2225	2230	rVB	38582	42789	1.15%	0.162%
29	15.556	2285	2290	2298	rBV	721967	931558	25.14%	3.537%
30	16.015	2363	2368	2376	rVB	55137	91093	2.46%	0.346%
31	16.533	2451	2456	2461	rBV2	50717	81344	2.20%	0.309%
32	17.145	2553	2560	2569	rBV6	35089	83863	2.26%	0.318%
33	17.862	2678	2682	2689	rVB3	29399	58425	1.58%	0.222%

Sum of corrected areas: 26336052

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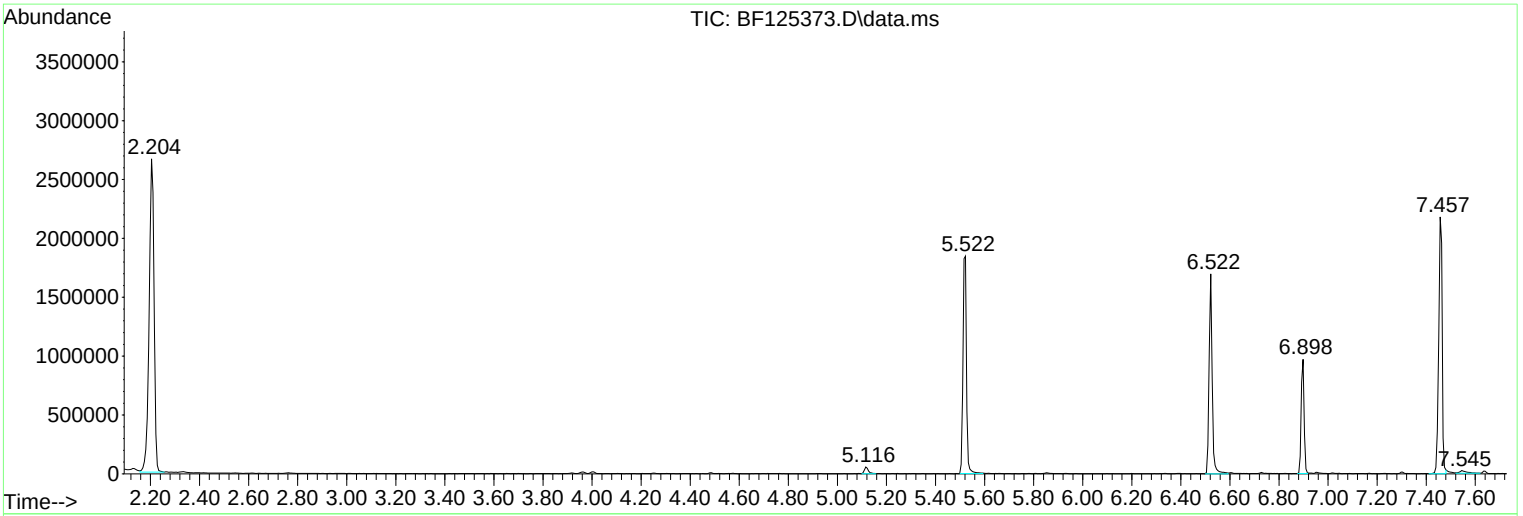
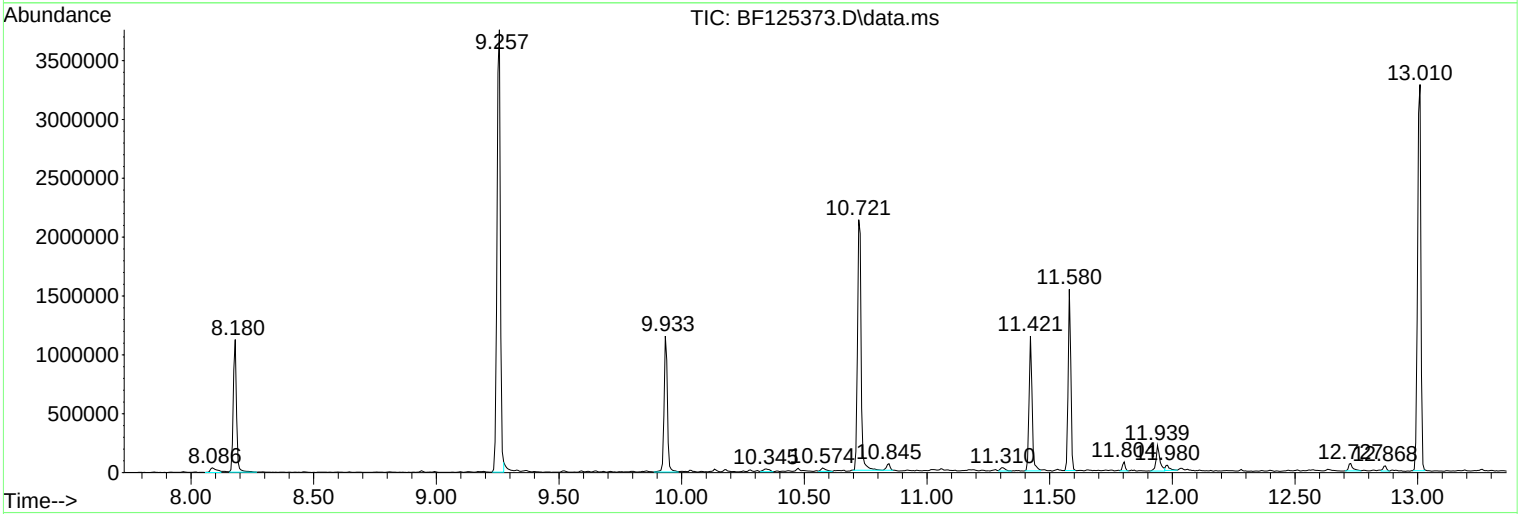
ALS Vial : 15 Sample Multiplier: 1

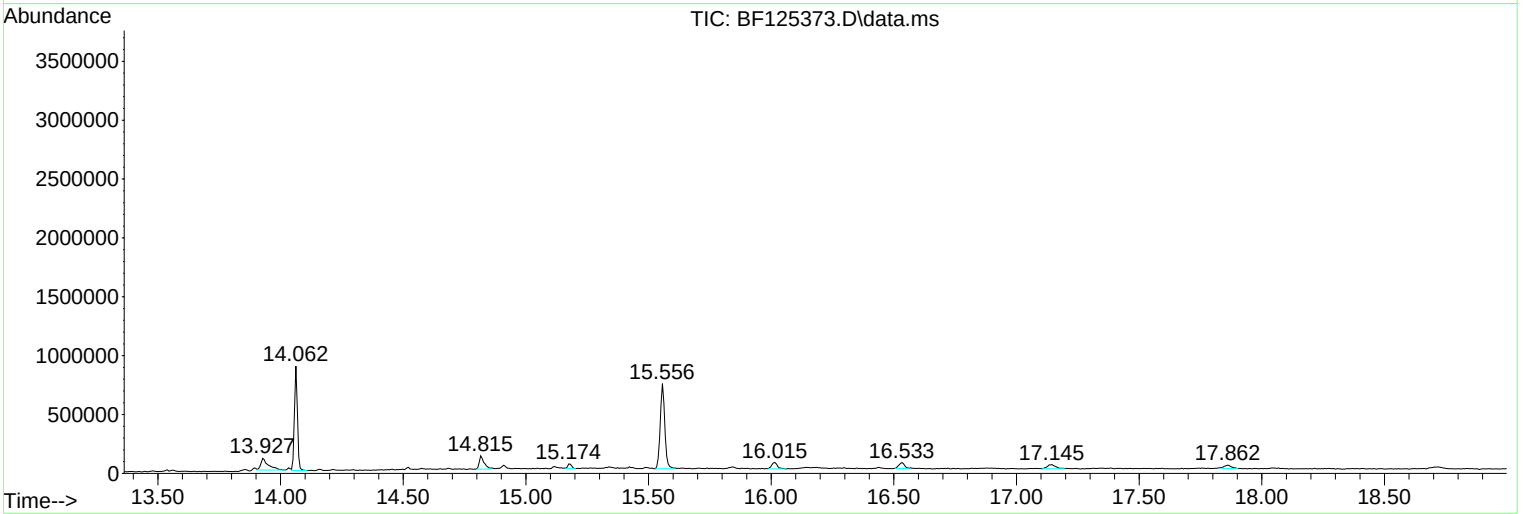
Instrument :
BNA_F
ClientSampleId :
20211059-SI-COMP-4-MODIFIED-EL

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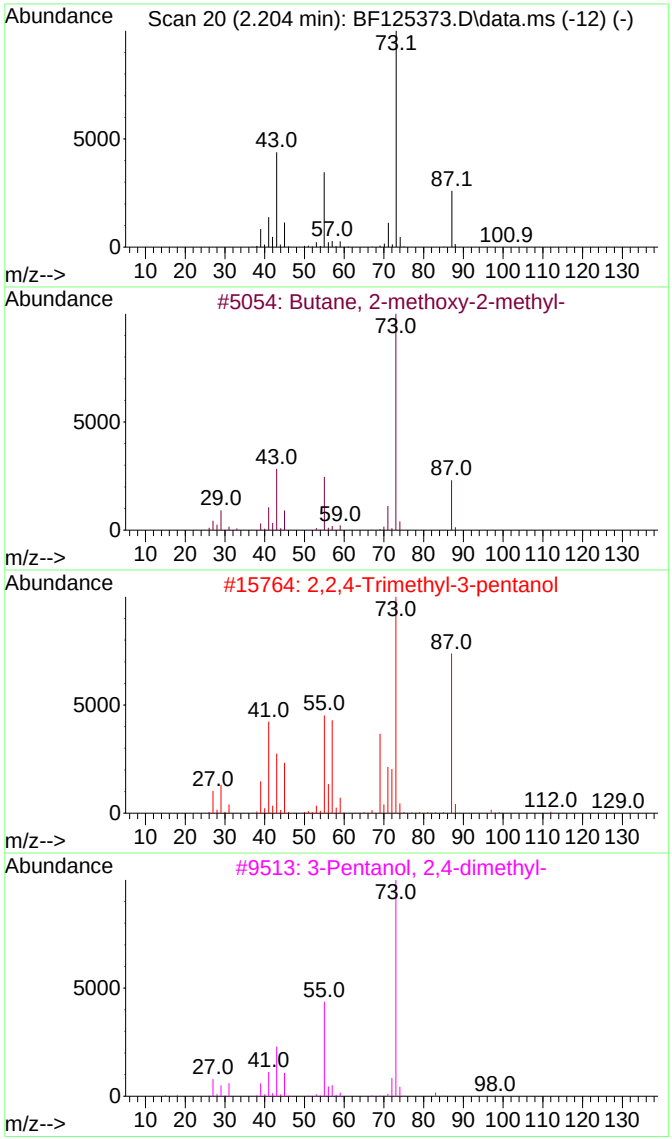
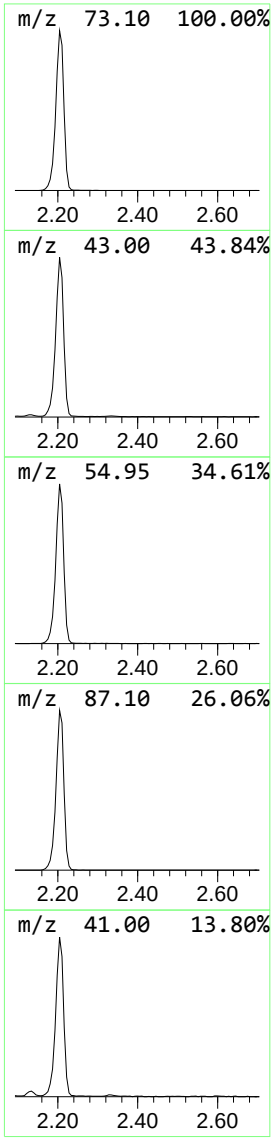
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	92.21 ng	3704820	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211059-SI-COMP-4-MODIFIED-EL

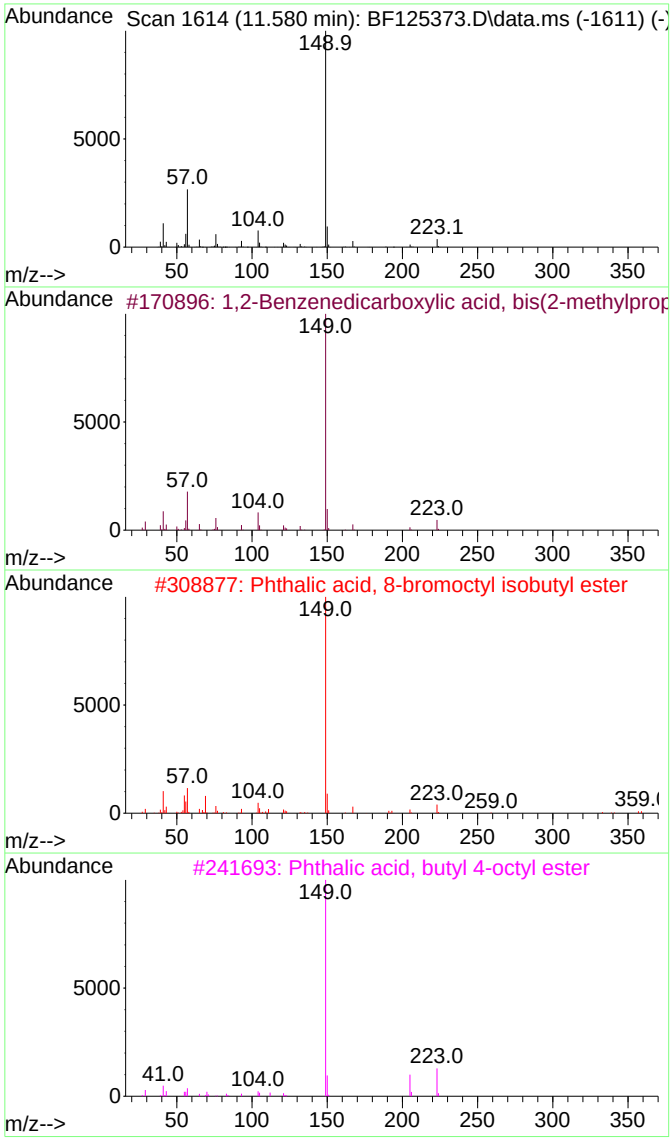
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

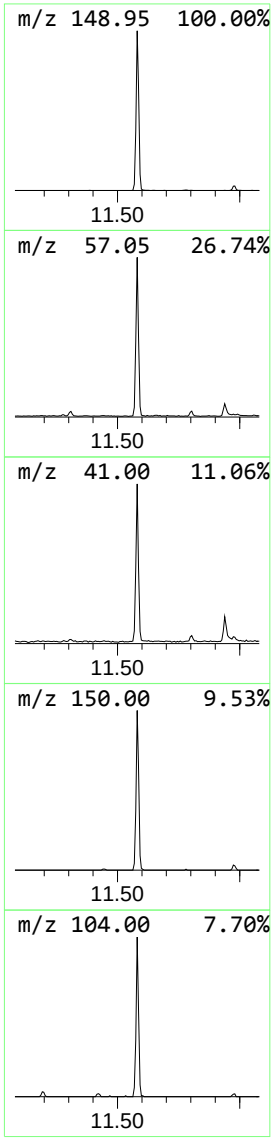
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	23.59 ng	1168430	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2	Phthalic acid, 8-bromoctyl isobu...	412	C20H29BrO4	1000382-55-3	83
3	Phthalic acid, butyl 4-octyl ester	334	C20H30O4	1000314-83-8	78
4	Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78
5	Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	78





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Sample : M3648-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211059-SI-COMP-4-MODIFIED-EL

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
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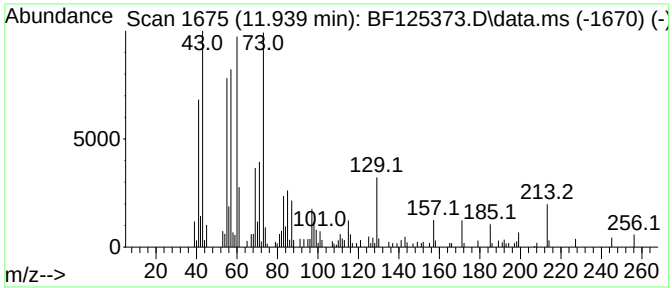
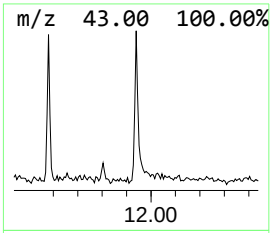
****

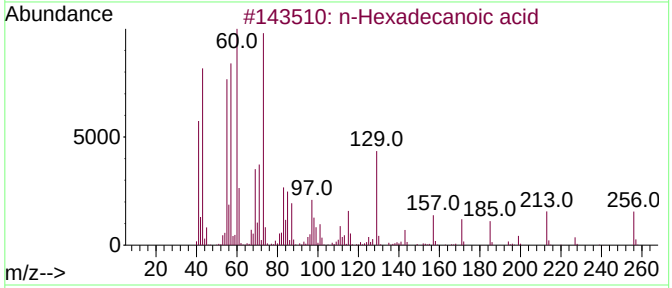
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

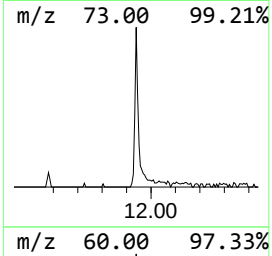
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	4.79 ng	237268	Phenanthrene-d10	11.421

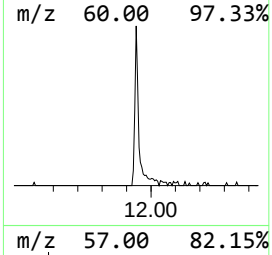
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78

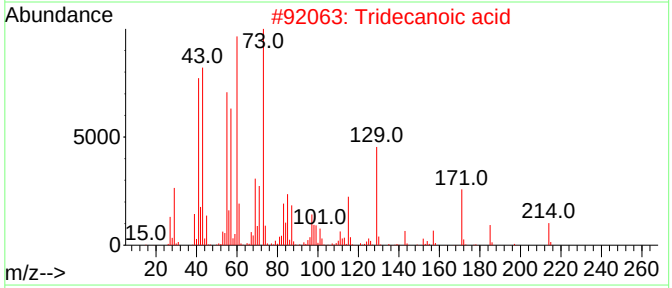


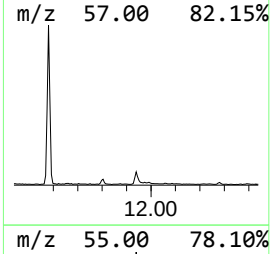


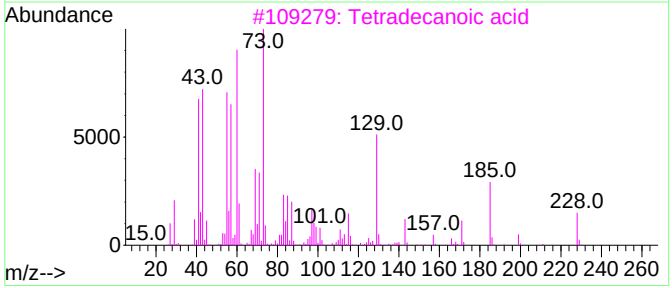


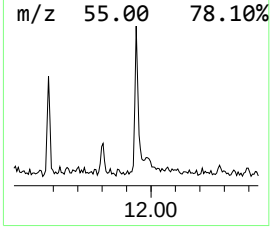












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20211059-SI-COMP-4-MODIFIED-EL

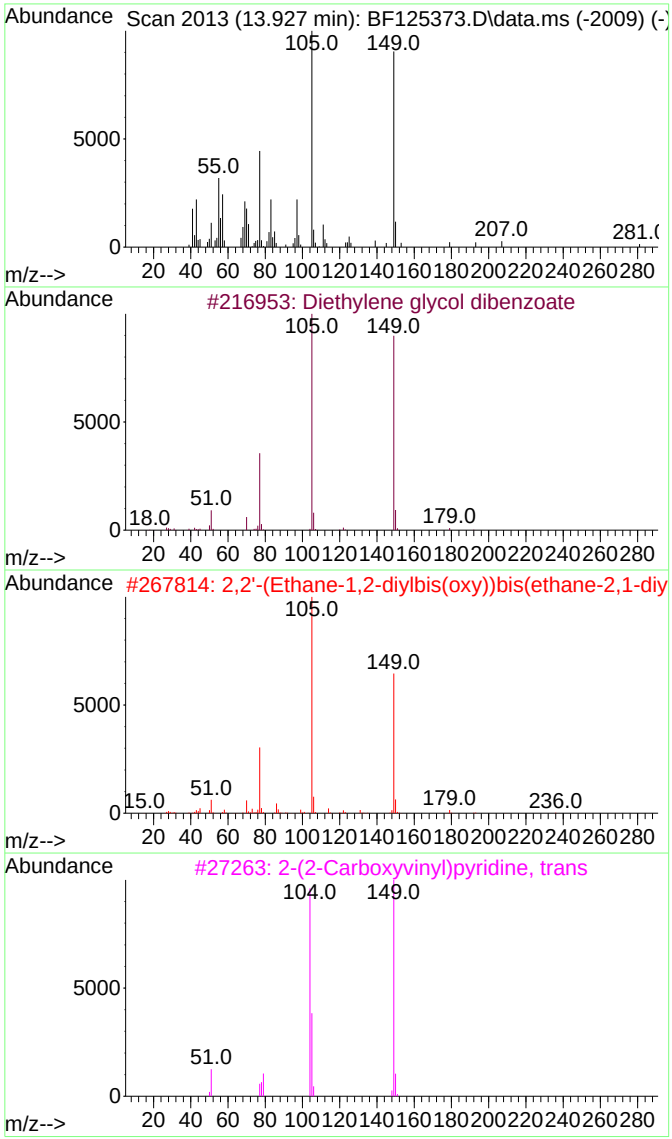
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

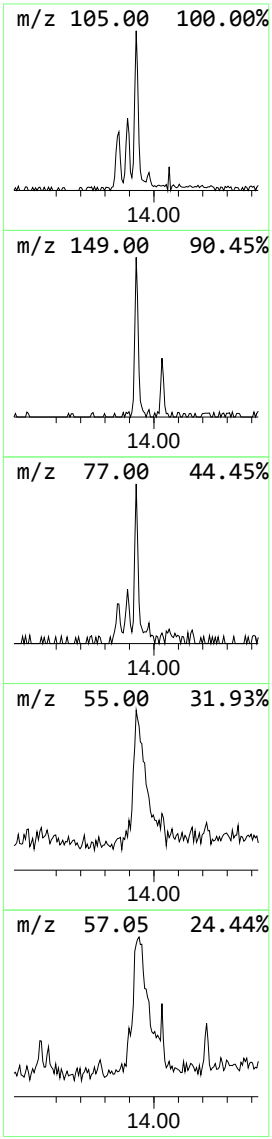
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	5.57 ng	213175	Chrysene-d12	14.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	53
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	43
4	Phthalic acid, 5-methoxy-3-methy...	322	C18H26O5	1010314-88-4	35
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	27





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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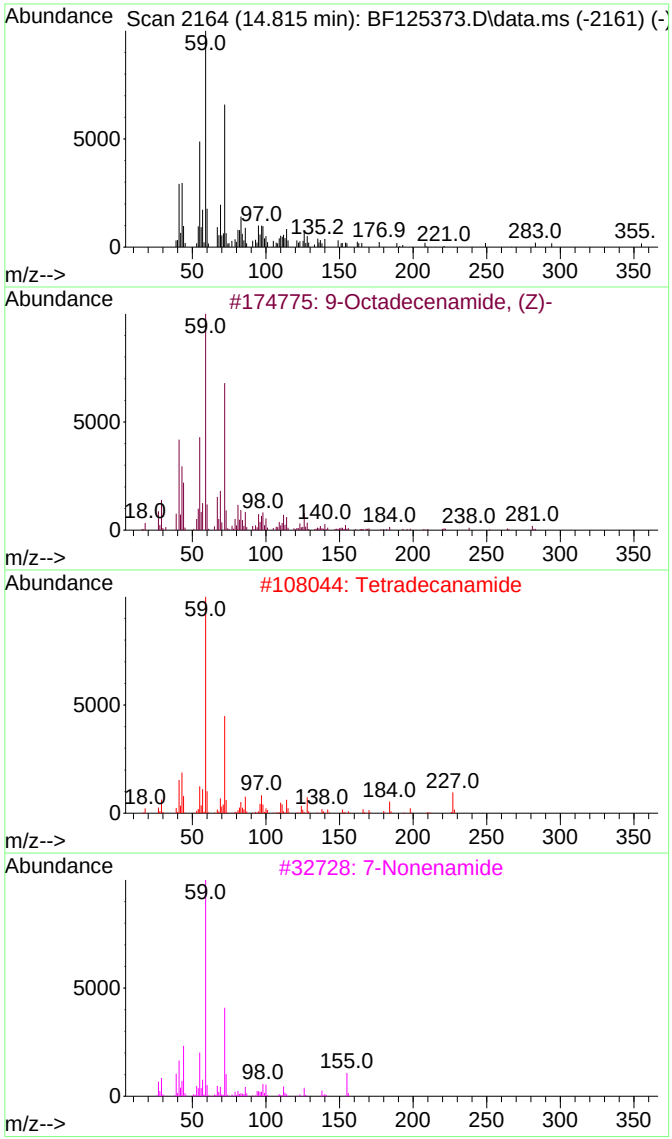
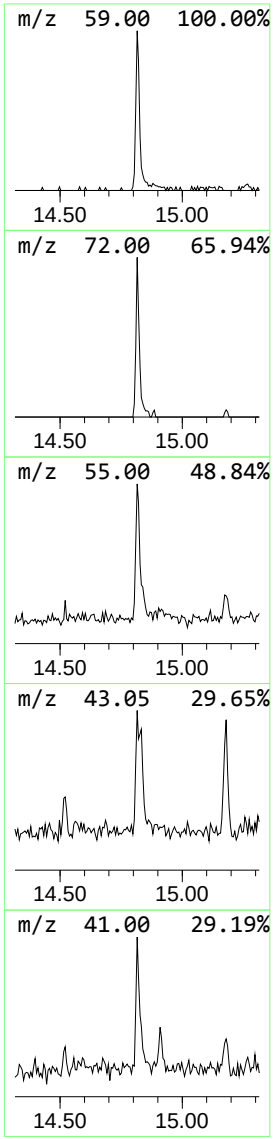
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	3.31 ng	154136	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	7-Nonenamide	155	C9H17NO	090949-53-4	64
4	Palmitoleamide	253	C16H31NO	106010-22-4	64
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	49





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.204	92.2	ng	3704820	1	6.898	803599	20.0
1,2-Benzenedica...	11.580	23.6	ng	1168430	4	11.421	990403	20.0
n-Hexadecanoic ...	11.939	4.8	ng	237268	4	11.421	990403	20.0
Diethylene glyc...	13.927	5.6	ng	213175	5	14.062	764829	20.0
9-Octadecenamid...	14.815	3.3	ng	154136	6	15.556	931558	20.0