LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
Data File : BF123978.D
Acq On : 18 May 2021 14:53
Operator : JU/CG
Sample : M2436-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1A

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123978.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	9	19	24	rBV	1033732	1340284	74.93%	9.750%
2	5.522	578	584	587	rBV	1577211	1664686	93.06%	12.110%
3	6.387	726	731	733	rBV2	50031	64687	3.62%	0.471%
4	6.528	750	755	758	rBV	1485882	1698717	94.96%	12.357%
5	6.728	786	789	795	rVB	43982	43418	2.43%	0.316%
6	6.904	815	819	822	rBV	427526	313989	17.55%	2.284%
7	7.469	908	915	918	rBV	1133091	1125077	62.90%	8.184%
8	8.186	1033	1037	1040	rBV	490106	384311	21.48%	2.796%
9	9.263	1216	1220	1223	rBV	2029497	1788800	100.00%	13.013%
10	9.657	1283	1287	1291	rBV	239224	210102	11.75%	1.528%
11	9.945	1332	1336	1339	rBV	581930	467776	26.15%	3.403%
12	10.351	1401	1405	1411	rVB2	25763	31377	1.75%	0.228%
13	10.416	1411	1416	1420	rBV2	30125	39056	2.18%	0.284%
14	10.733	1465	1470	1473	rBV	1620927	1384669	77.41%	10.073%
15	10.863	1487	1492	1495	rBV4	30297	31641	1.77%	0.230%
16	11.174	1542	1545	1549	rVB	59606	60891	3.40%	0.443%
17	11.327	1568	1571	1573	rVB3	28852	26190	1.46%	0.191%
18	11.427	1585	1588	1592	rBV	514953	479493	26.81%	3.488%
19	11.810	1650	1653	1658	rVB7	43878	47232	2.64%	0.344%
20	11.874	1662	1664	1668	rBV4	24386	33184	1.86%	0.241%
21	11.957	1674	1678	1681	rBV	204277	189059	10.57%	1.375%
22	12.192	1716	1718	1725	rBV8	28906	39617	2.21%	0.288%
23	12.416	1753	1756	1761	rBV7	34637	64442	3.60%	0.469%
24	13.021	1854	1859	1862	rBV	1518024	1379499	77.12%	10.035%
25	13.921	2009	2012	2018	rVB3	184564	222551	12.44%	1.619%
26	14.074	2035	2038	2041	rBV	292157	259132	14.49%	1.885%
27	14.545	2116	2118	2124	rBV5	78392	105391	5.89%	0.767%
28	15.568	2289	2292	2296	rVB	208205	251179	14.04%	1.827%

Sum of corrected areas: 13746450

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Misc :
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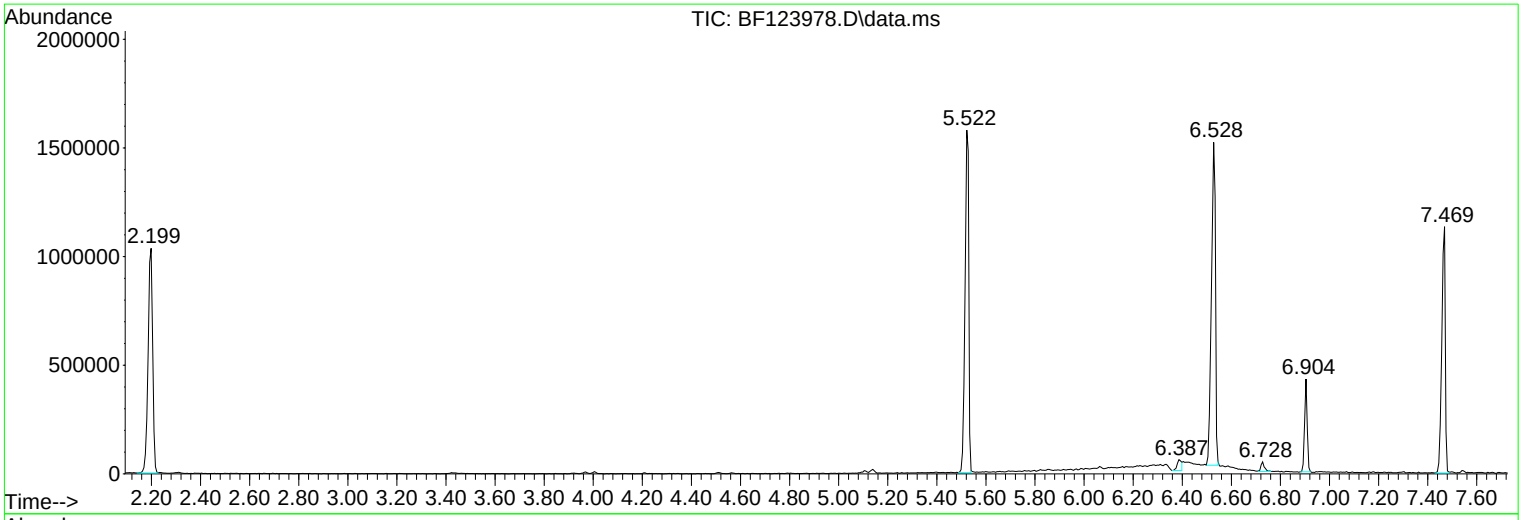
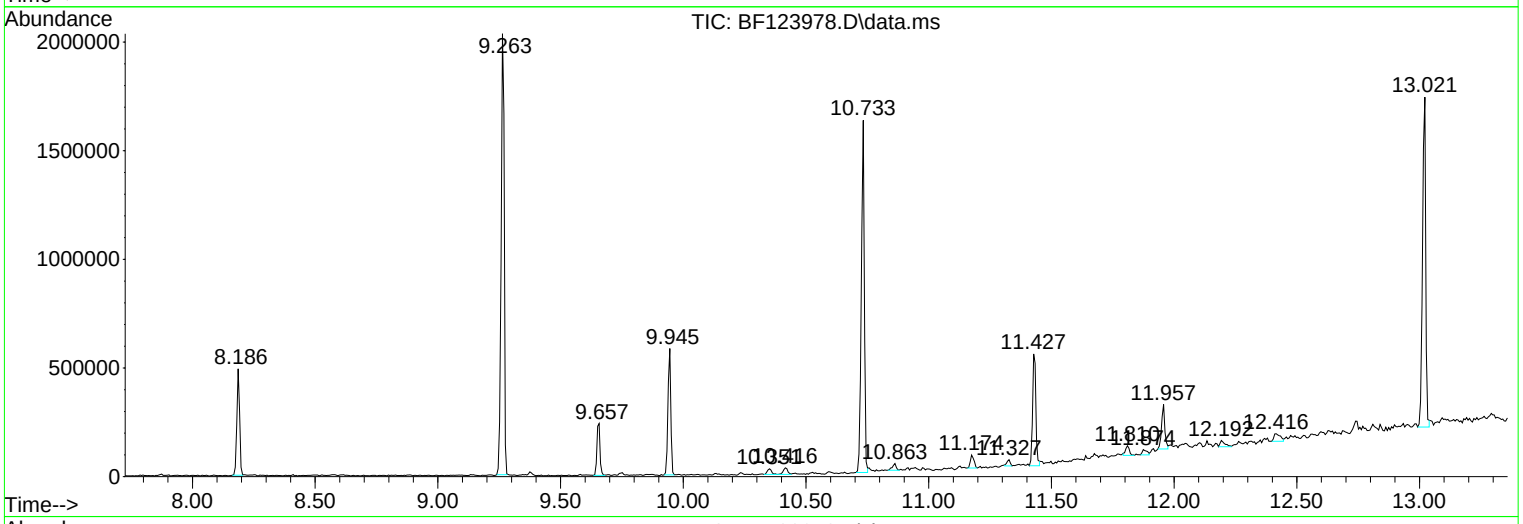
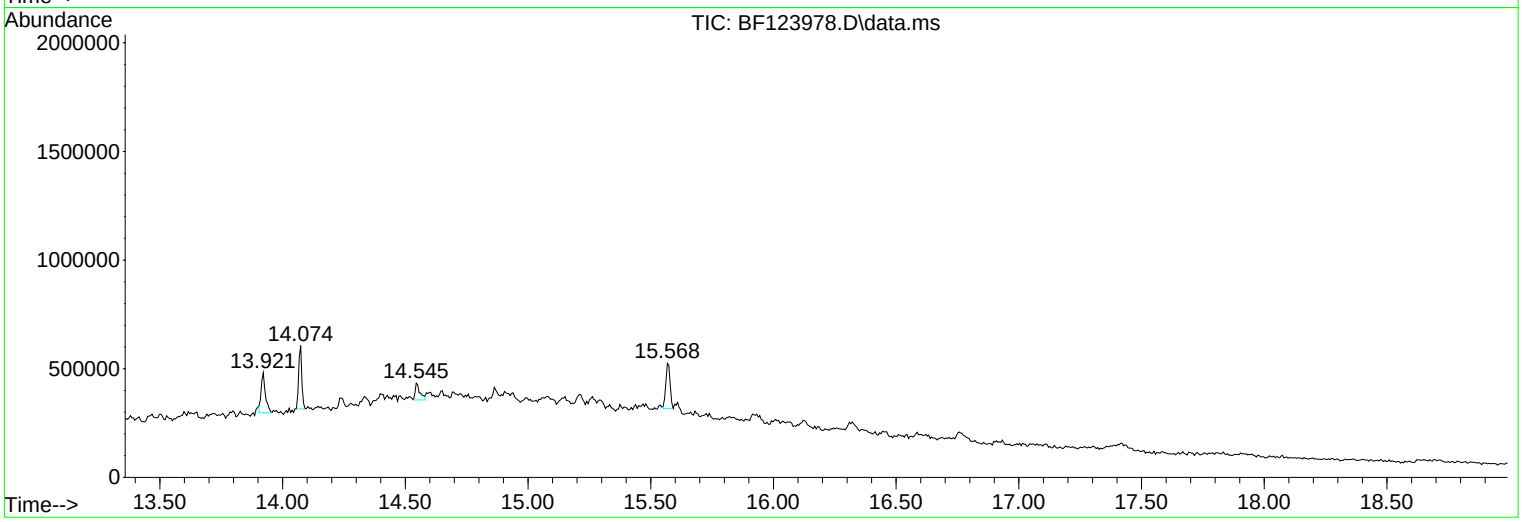
Instrument :
BNA_F
ClientSampleId :
TP-1A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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ClientSampleId :
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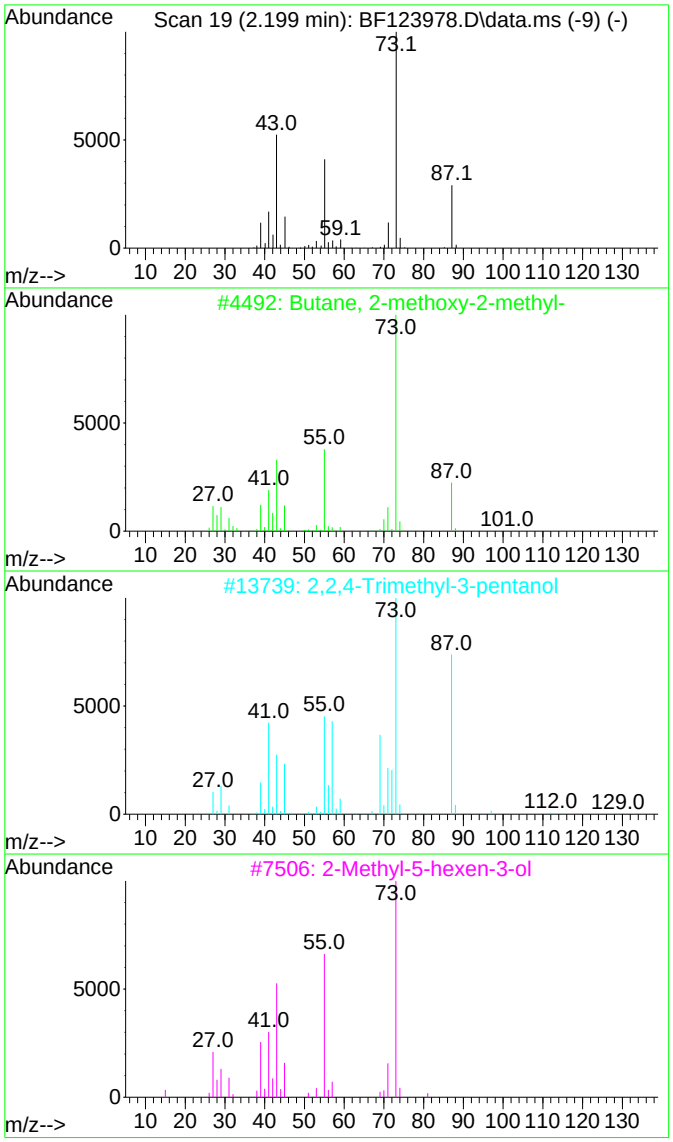
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

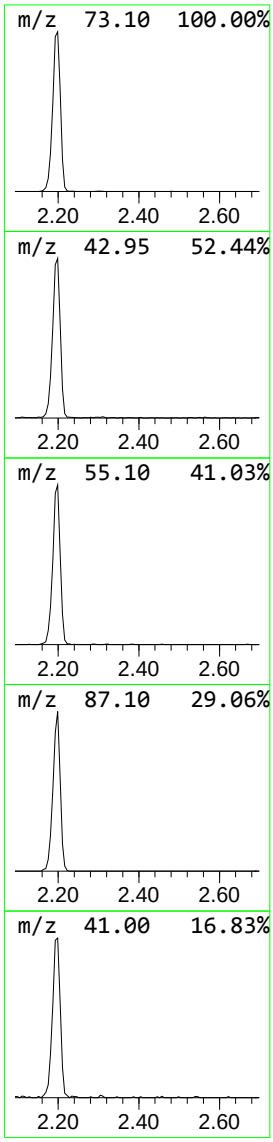
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	85.37 ng	1340280	1,4-Dichlorobenzene-d4	6.904

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	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9





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Data File : BF123978.D
Acq On : 18 May 2021 14:53
Operator : JU/CG
Sample : M2436-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1A

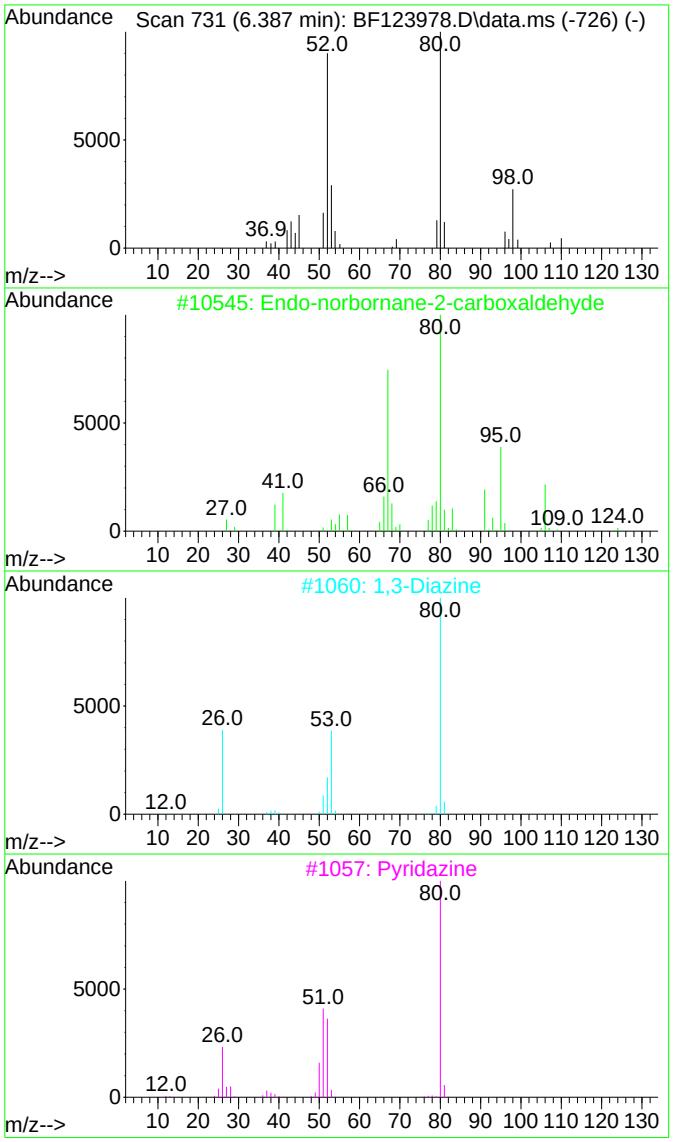
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

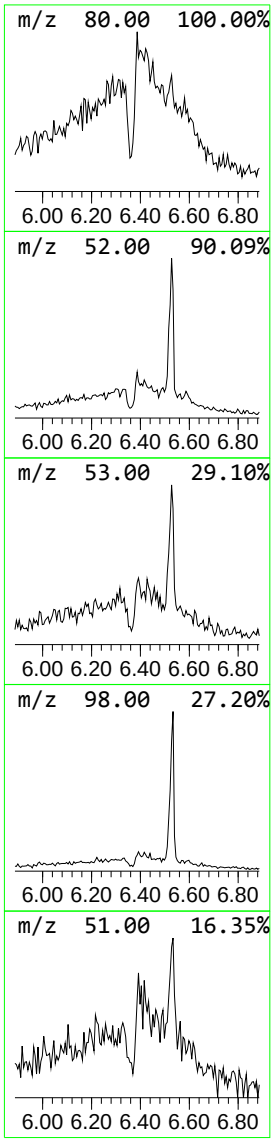
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown6.387 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.387	4.12 ng	64687	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Endo-norbornane-2-carboxaldehyde	124	C8H12O	003574-54-7	17
2	1,3-Diazine	80	C4H4N2	000289-95-2	9
3	Pyridazine	80	C4H4N2	000289-80-5	9
4	2-Hexen-4-yne, (E)-	80	C6H8	033625-96-6	9
5	2-Hexen-4-yne, (Z)-	80	C6H8	030626-48-3	9





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ClientSampleId :
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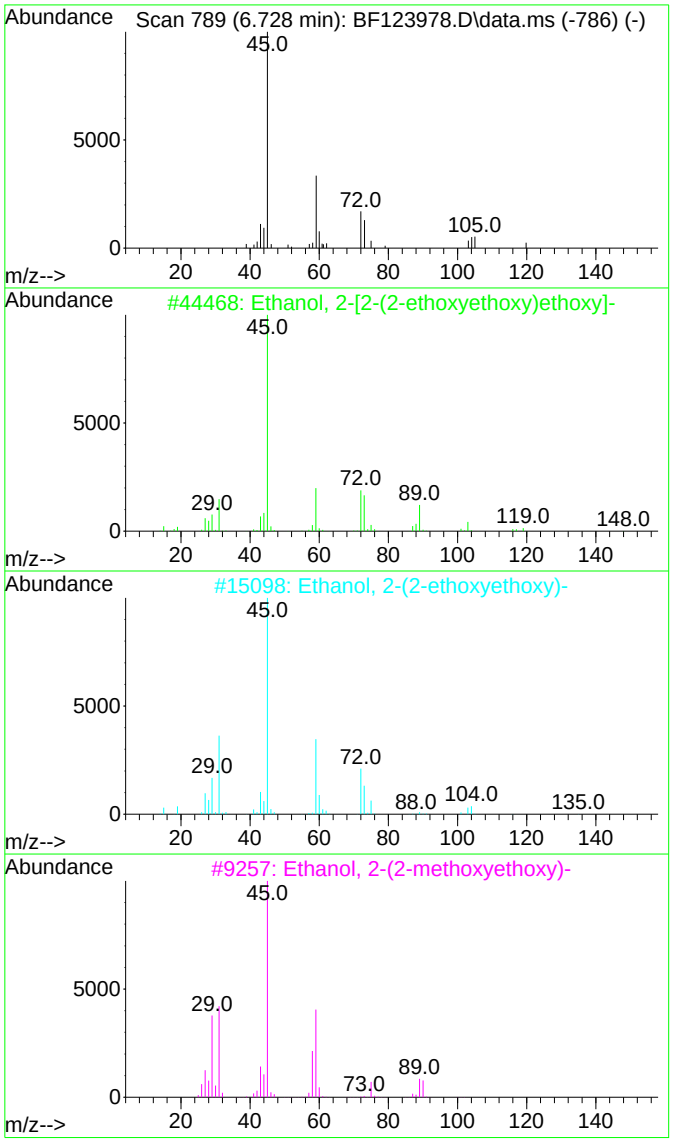
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

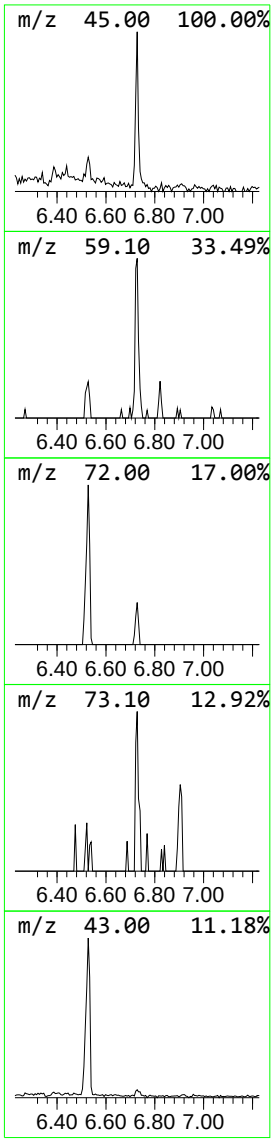
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-[2-(2-ethoxyetho... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	2.77 ng	43418	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	56
2	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	47
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	38
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	33





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Data File : BF123978.D
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Operator : JU/CG
Sample : M2436-01
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Instrument :
BNA_F
ClientSampleId :
TP-1A

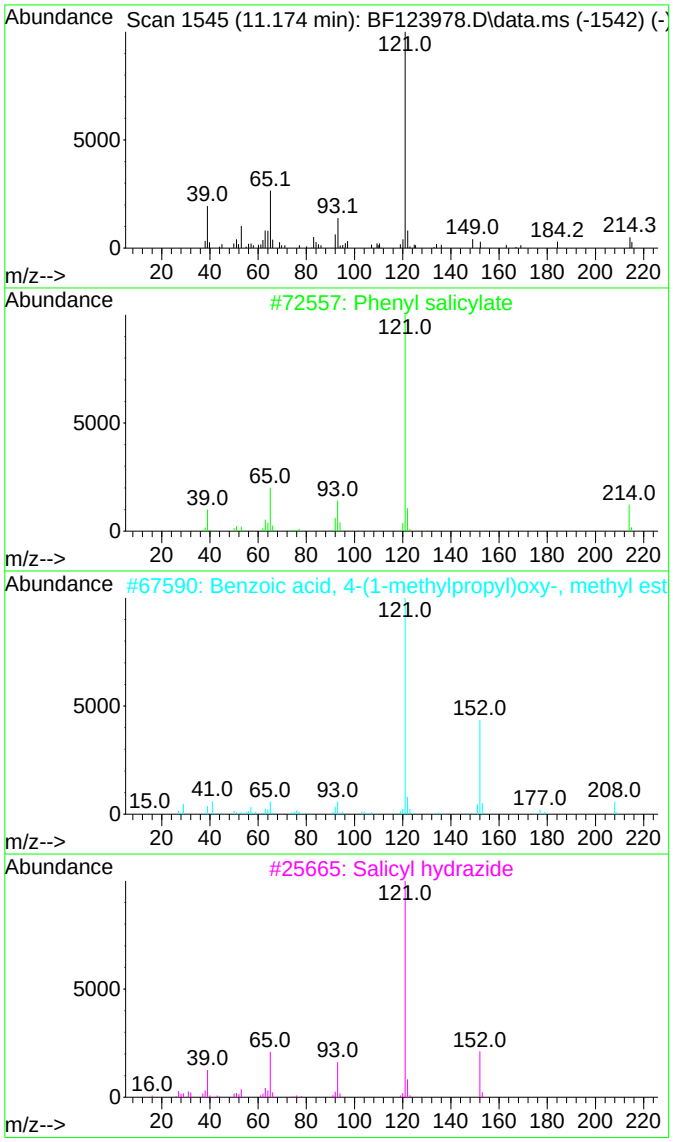
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

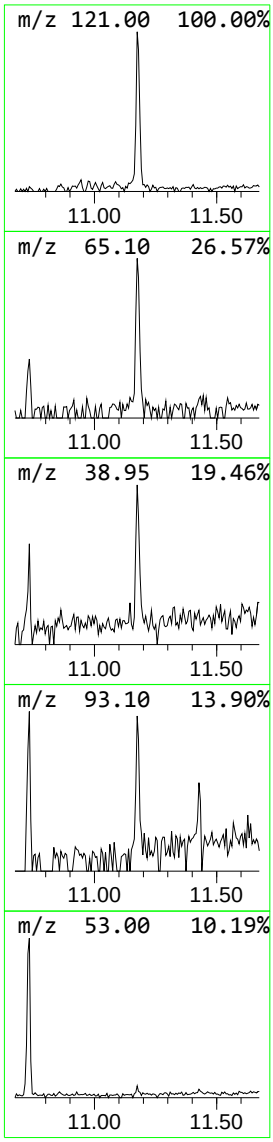
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenyl salicylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.175	2.54 ng	60891	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl salicylate	214	C13H10O3	000118-55-8	90
2	Benzoic acid, 4-(1-methylpropyl)...	208	C12H16O3	1000375-32-9	72
3	Salicyl hydrazide	152	C7H8N2O2	000936-02-7	72
4	Salicylhydrazide, N2-phenylsulfo...	292	C13H12N2O4S	1000294-09-9	72
5	2-Pyrazolin-5-ol, 5-tridecafluor...	538	C17H11F13N2O3	1000264-75-0	72





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

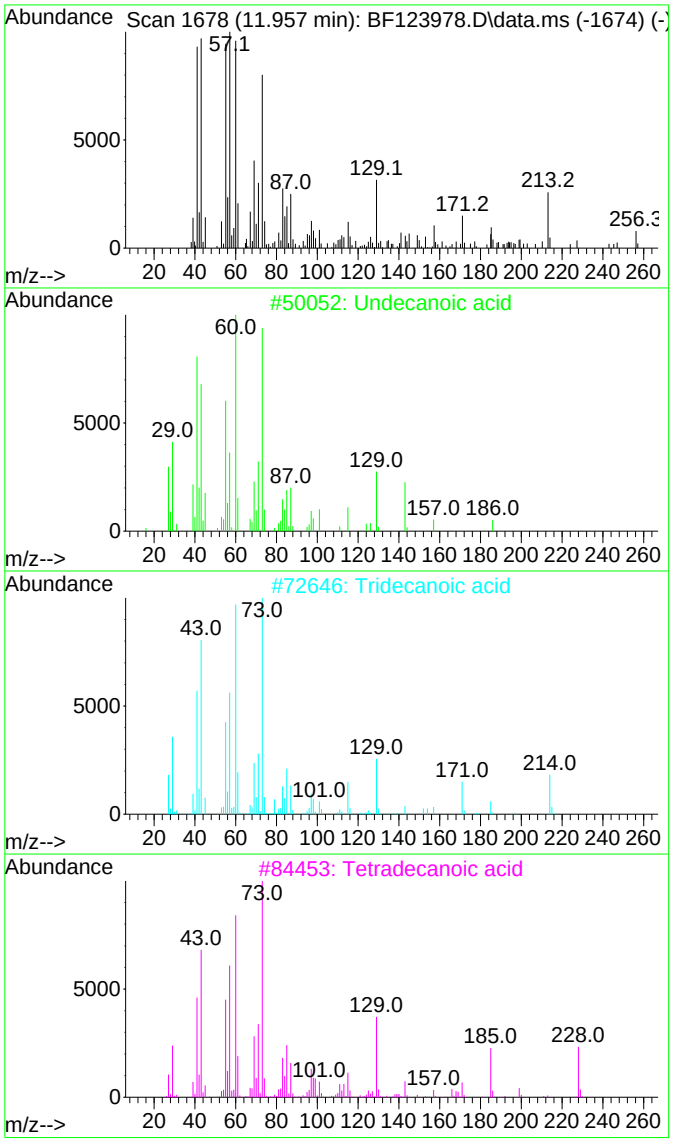
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

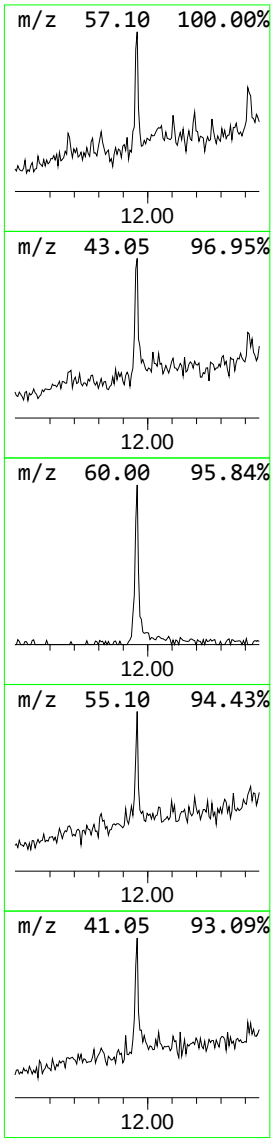
****

Peak Number 5 Undecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	7.89 ng	189059	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





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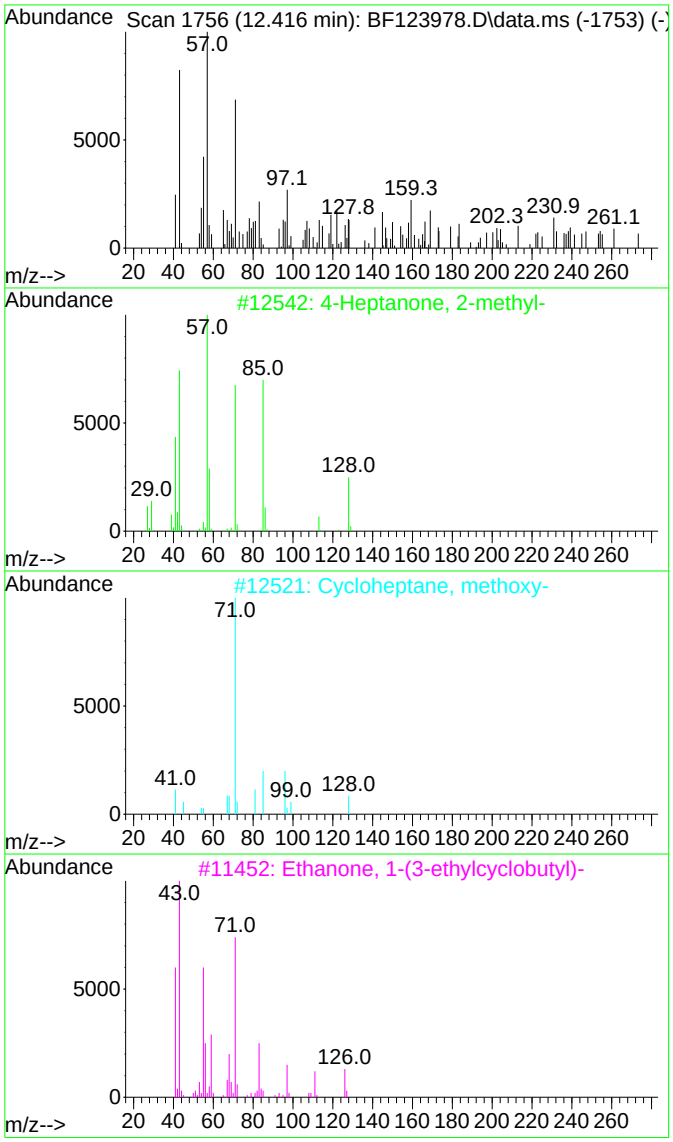
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

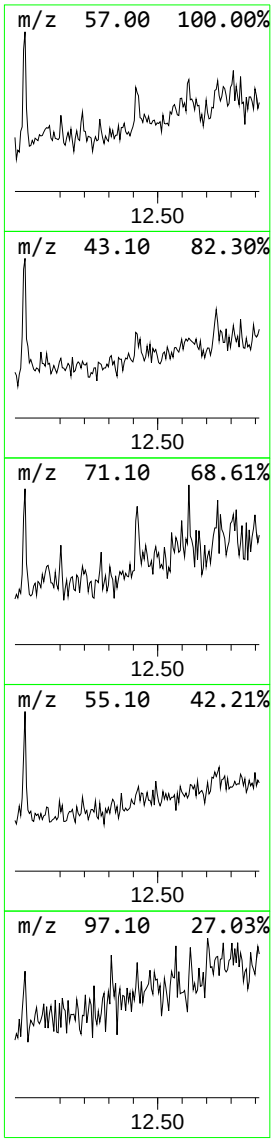
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown12.416 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	2.69 ng	64442	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	27
2	Cycloheptane, methoxy-	128	C8H16O	042604-04-6	25
3	Ethanone, 1-(3-ethylcyclobutyl)-	126	C8H14O	056335-71-8	22
4	Butanoic acid, 2-chlorophenyl ester	198	C10H11ClO2	063867-11-8	16
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	14





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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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TIC Library : C:\DATABASE\NIST11.L
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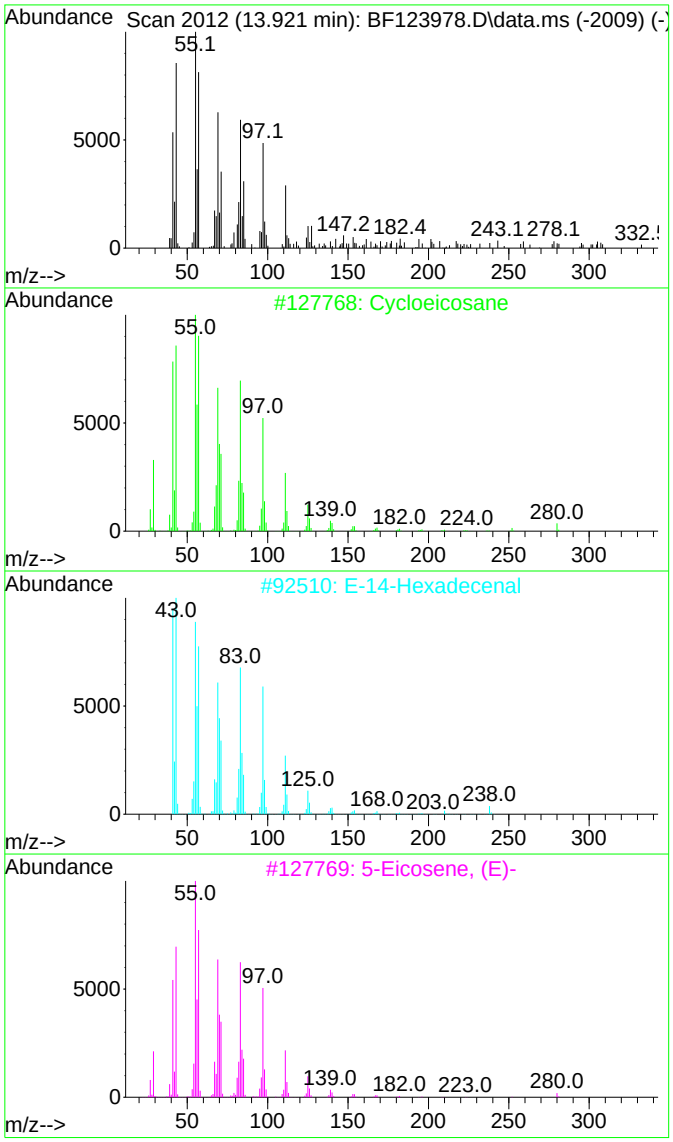
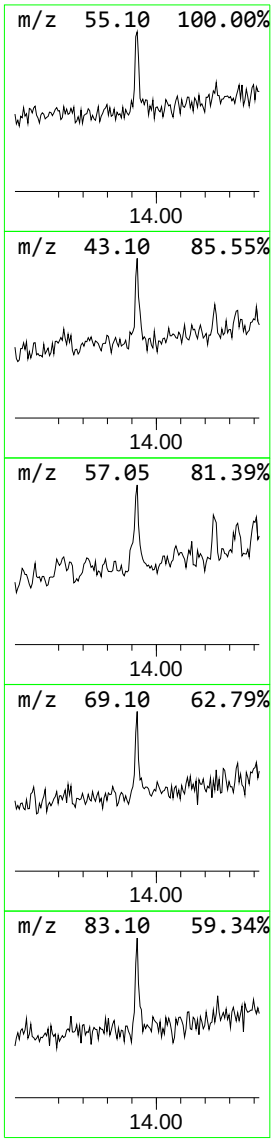
****

Peak Number 7 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	17.18 ng	222551	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	93
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	89
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4	1-Docosene	308	C22H44	001599-67-3	83
5	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	83





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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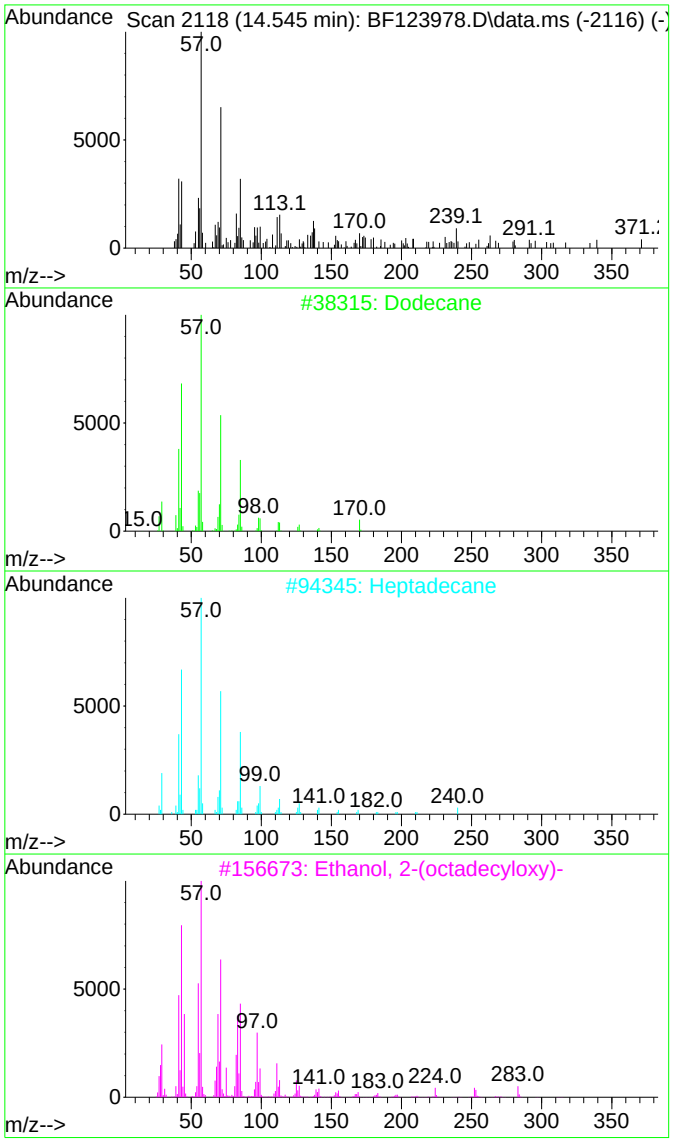
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

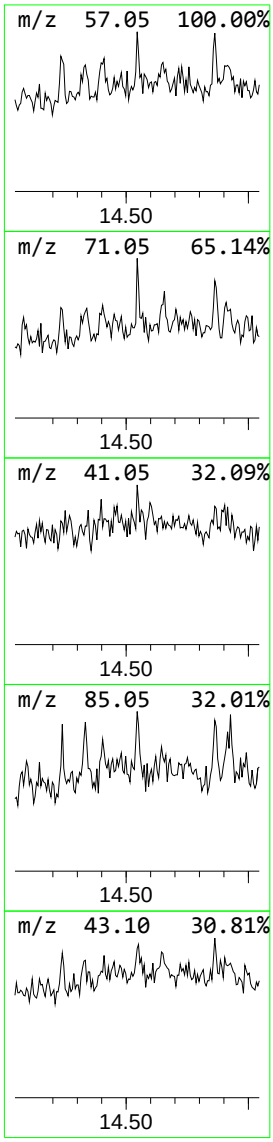
****

Peak Number 8 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	8.13 ng	105391	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	55
2	Heptadecane	240	C17H36	000629-78-7	55
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	43
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	43
5	Decane, 2-methyl-	156	C11H24	006975-98-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
Data File : BF123978.D
Acq On : 18 May 2021 14:53
Operator : JU/CG
Sample : M2436-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.199	85.4	ng	1340280	1	6.904	313989	20.0
unknown6.387	6.387	4.1	ng	64687	1	6.904	313989	20.0
Ethanol, 2-[2-(...	6.728	2.8	ng	43418	1	6.904	313989	20.0
Phenyl salicylate	11.175	2.5	ng	60891	4	11.427	479493	20.0
Undecanoic acid	11.957	7.9	ng	189059	4	11.427	479493	20.0
unknown12.416	12.416	2.7	ng	64442	4	11.427	479493	20.0
Cycloeicosane	13.921	17.2	ng	222551	5	14.074	259132	20.0
Dodecane	14.545	8.1	ng	105391	5	14.074	259132	20.0