LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 55-ST-34

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	27	33	40	rVB	1357645	1805595	33.25%	3.990%
2	5.569	588	592	595	rBV	2252743	1928687	35.51%	4.262%
3	6.563	757	761	766	rBV	1527478	1278991	23.55%	2.826%
4	6.928	810	823	824	rBV	78983	196740	3.62%	0.435%
5	6.957	824	828	831	rVB	1213988	1129317	20.79%	2.495%
6	7.039	836	842	849	rBV2	93824	179095	3.30%	0.396%
7	7.351	890	895	898	rVB3	44020	60113	1.11%	0.133%
8	7.516	918	923	926	rBV	3509802	3704516	68.21%	8.186%
9	7.563	926	931	934	rBV2	54849	58766	1.08%	0.130%
10	7.686	947	952	958	rBV3	75354	151851	2.80%	0.336%
11	7.745	958	962	975	rVB6	200519	594641	10.95%	1.314%
12	7.898	982	988	992	rBV6	25038	62518	1.15%	0.138%
13	7.963	993	999	1002	rVV3	151058	304635	5.61%	0.673%
14	8.022	1002	1009	1010	rVV5	189291	460860	8.49%	1.018%
15	8.075	1013	1018	1021	rVV2	497166	1023045	18.84%	2.261%
16	8.104	1021	1023	1027	rVV	272569	485546	8.94%	1.073%
17	8.180	1027	1036	1038	rVV2	701054	1819844	33.51%	4.021%
18	8.233	1040	1045	1049	rVV2	2062991	3569460	65.72%	7.887%
19	8.286	1049	1054	1057	rVV2	1126676	1866566	34.37%	4.124%
20	8.398	1060	1073	1076	rVV2	1764848	4301291	79.20%	9.504%
21	8.422	1076	1077	1079	rVV2	231349	158866	2.93%	0.351%
22	8.445	1079	1081	1083	rVV2	232766	191318	3.52%	0.423%
23	8.469	1083	1085	1088	rVV3	171694	170201	3.13%	0.376%
24	8.522	1091	1094	1095	rVV2	151937	152949	2.82%	0.338%
25	8.539	1095	1097	1100	rVV2	183098	215156	3.96%	0.475%
26	8.569	1100	1102	1103	rVV2	169668	158716	2.92%	0.351%
27	8.592	1103	1106	1108	rVV2	212887	297698	5.48%	0.658%
28	8.616	1108	1110	1114	rVV3	253726	293425	5.40%	0.648%
29	8.663	1114	1118	1120	rVV2	278210	330042	6.08%	0.729%
30	8.686	1120	1122	1127	rVV4	239471	338184	6.23%	0.747%
31	8.757	1130	1134	1139	rVV2	161352	214445	3.95%	0.474%
32	8.827	1139	1146	1149	rVB4	168196	296363	5.46%	0.655%
33	8.892	1154	1157	1162	rBV4	55520	74206	1.37%	0.164%
34	9.316	1223	1229	1232	rBV	5919084	5431024	100.00%	12.001%
35	9.798	1306	1311	1314	rBV	125316	158009	2.91%	0.349%
36	9.998	1339	1345	1348	rBV	1808877	1631604	30.04%	3.605%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.127	1364	1367	1375	rVB	77895	79118	1.46%	0.175%
38	10.786	1475	1479	1482	rBV	2512415	2160812	39.79%	4.775%
39	11.486	1594	1598	1602	rBV	1596737	1364789	25.13%	3.016%
40	11.998	1682	1685	1695	rBV2	131157	173633	3.20%	0.384%
41	12.715	1801	1807	1813	rBV7	38492	85618	1.58%	0.189%
42	12.792	1817	1820	1828	rVV	74424	93235	1.72%	0.206%
43	13.080	1864	1869	1872	rBV	4712043	4125903	75.97%	9.117%
44	13.992	2022	2024	2033	rVB3	38951	72397	1.33%	0.160%
45	14.133	2045	2048	2052	rBV	1046703	902551	16.62%	1.994%
46	15.656	2302	2307	2315	rBV2	796384	1103238	20.31%	2.438%

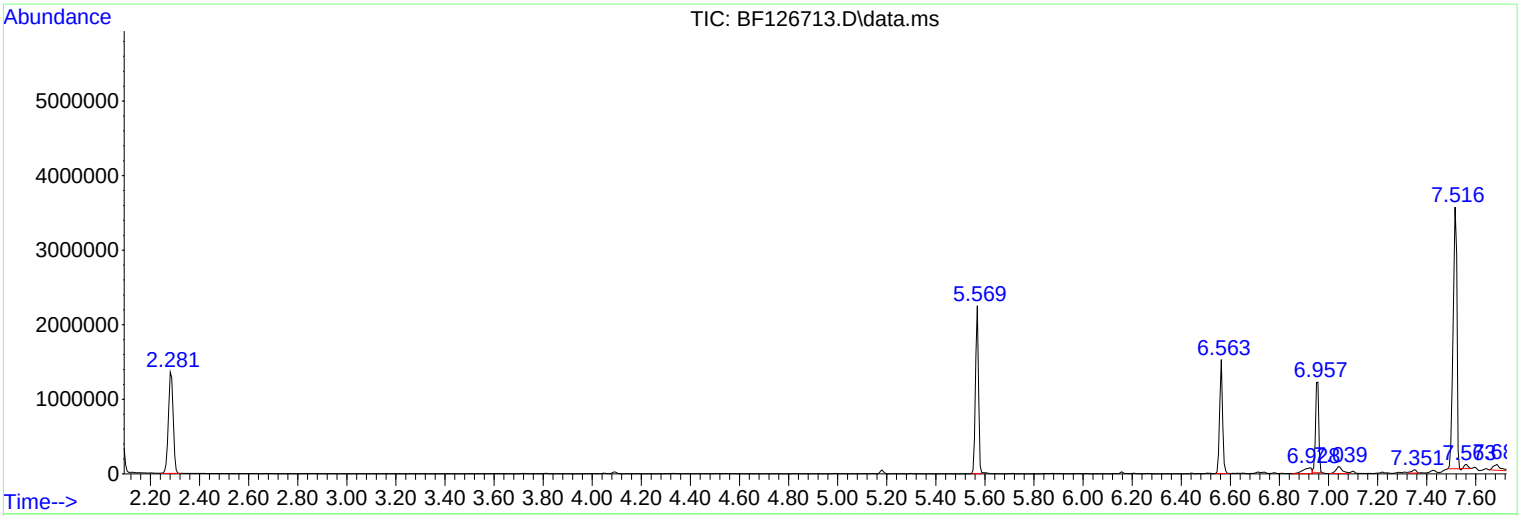
Sum of corrected areas: 45255577

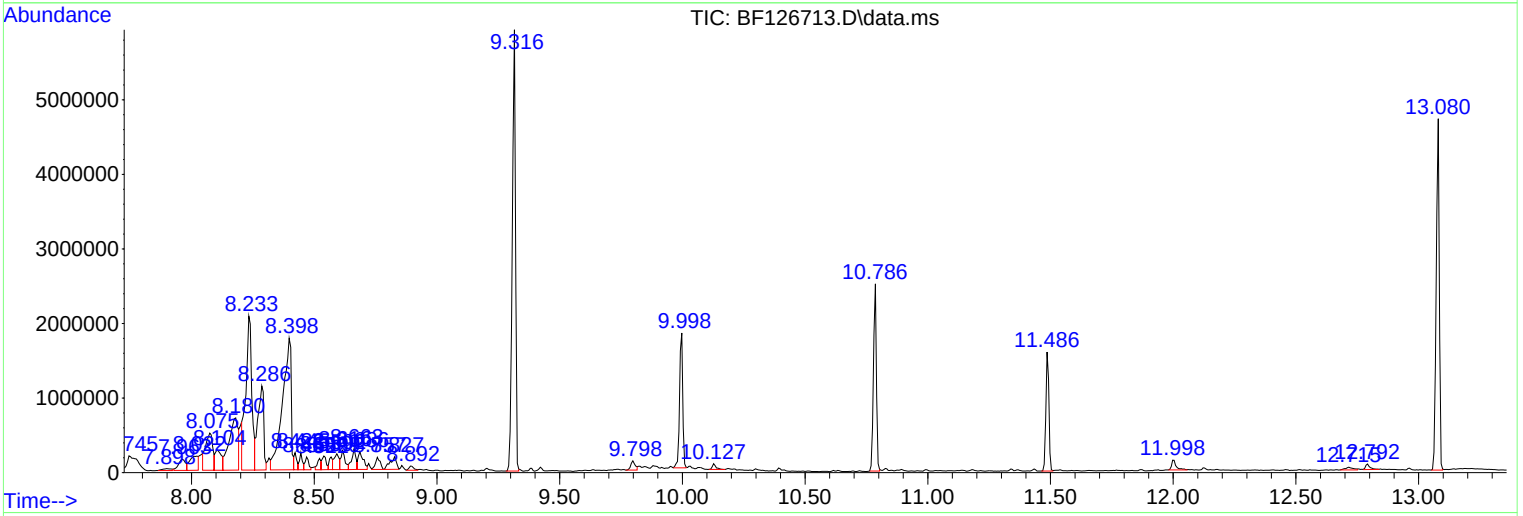
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

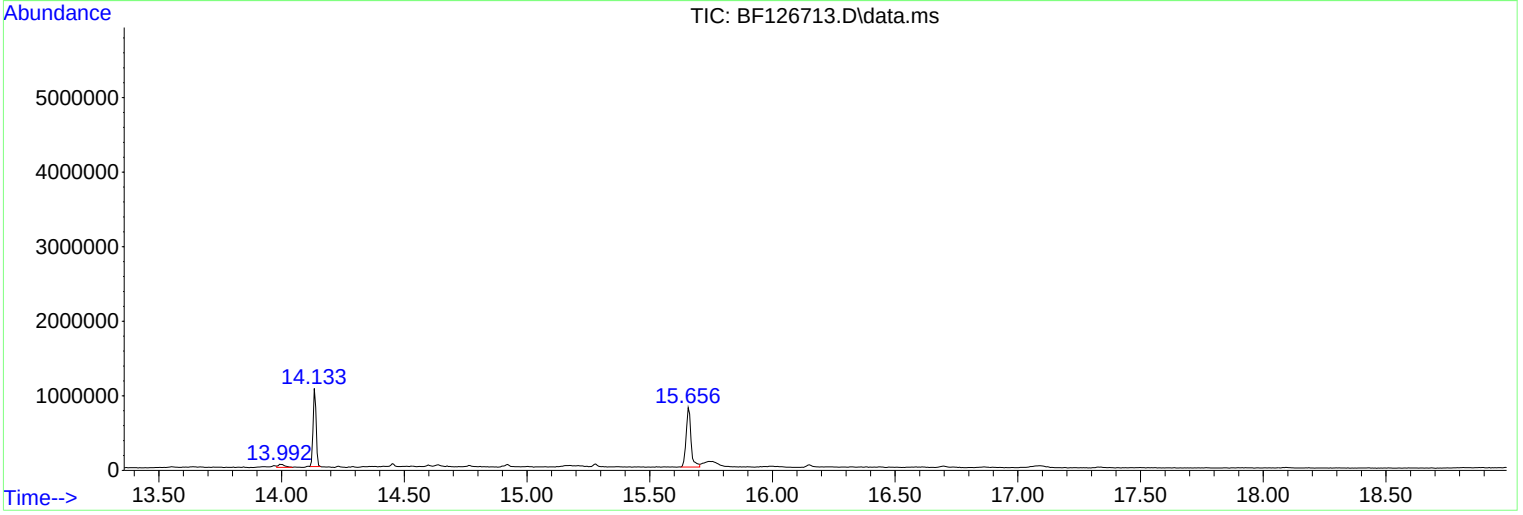
Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

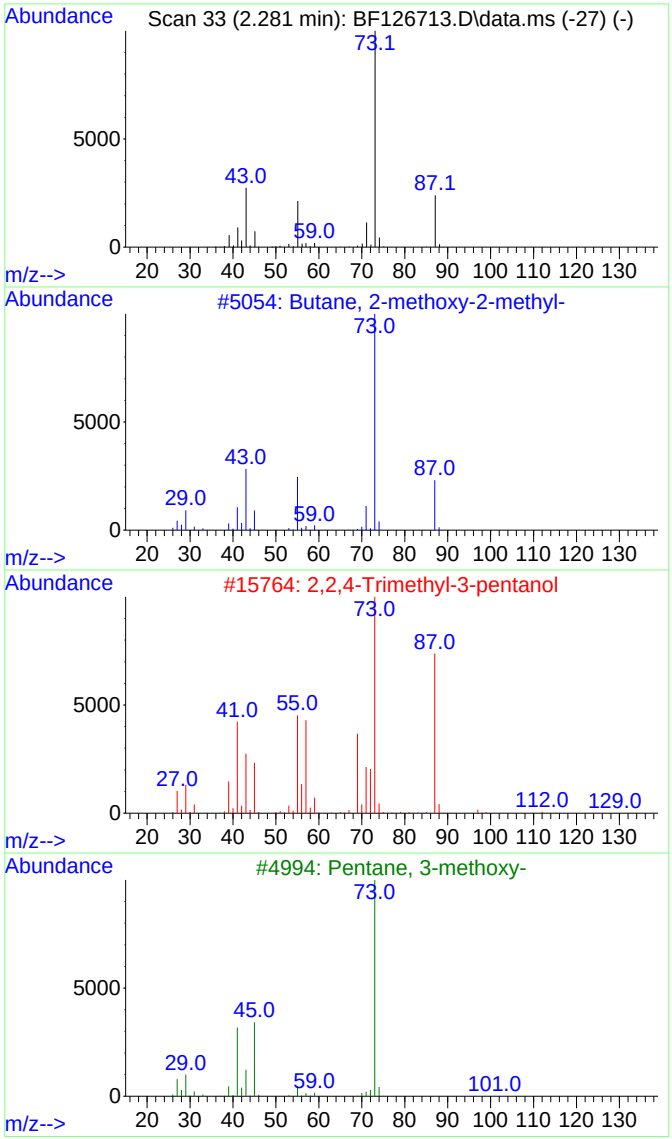
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

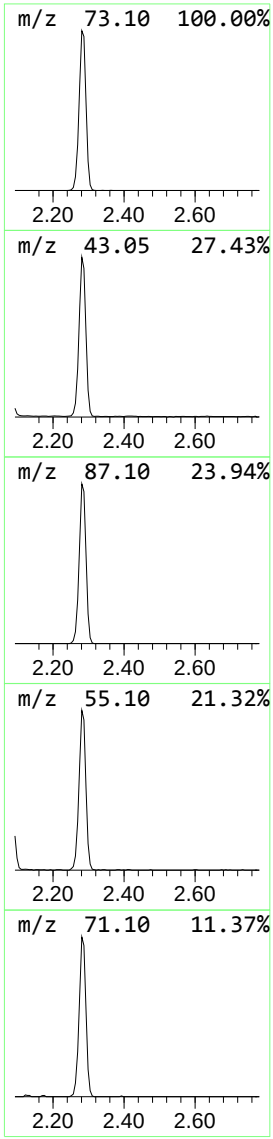
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	31.98 ng	1805600	1,4-Dichlorobenzene-d4	6.957

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

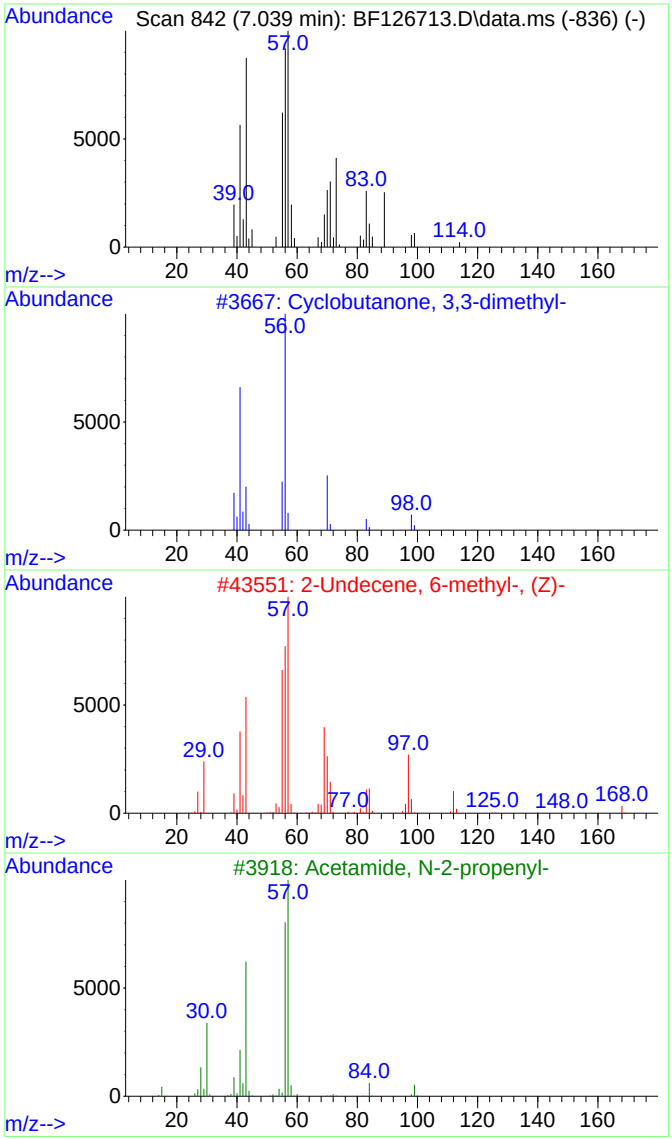
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

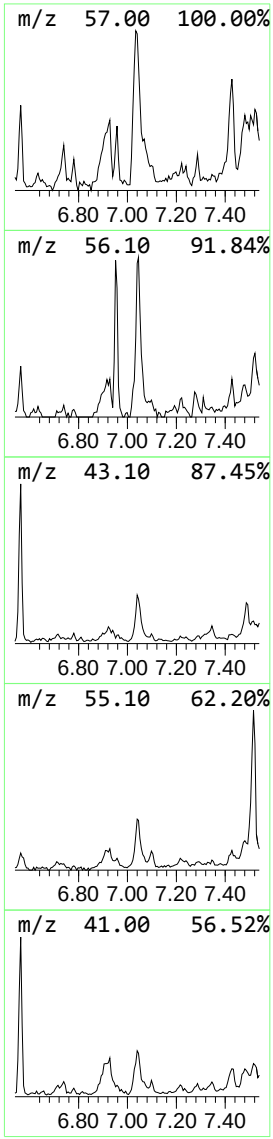
****

Peak Number 2 unknown7.039 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.039	3.17 ng	179095	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	43
2	2-Undecene, 6-methyl-, (Z)-	168	C12H24	074630-43-6	40
3	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	38
4	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	38
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

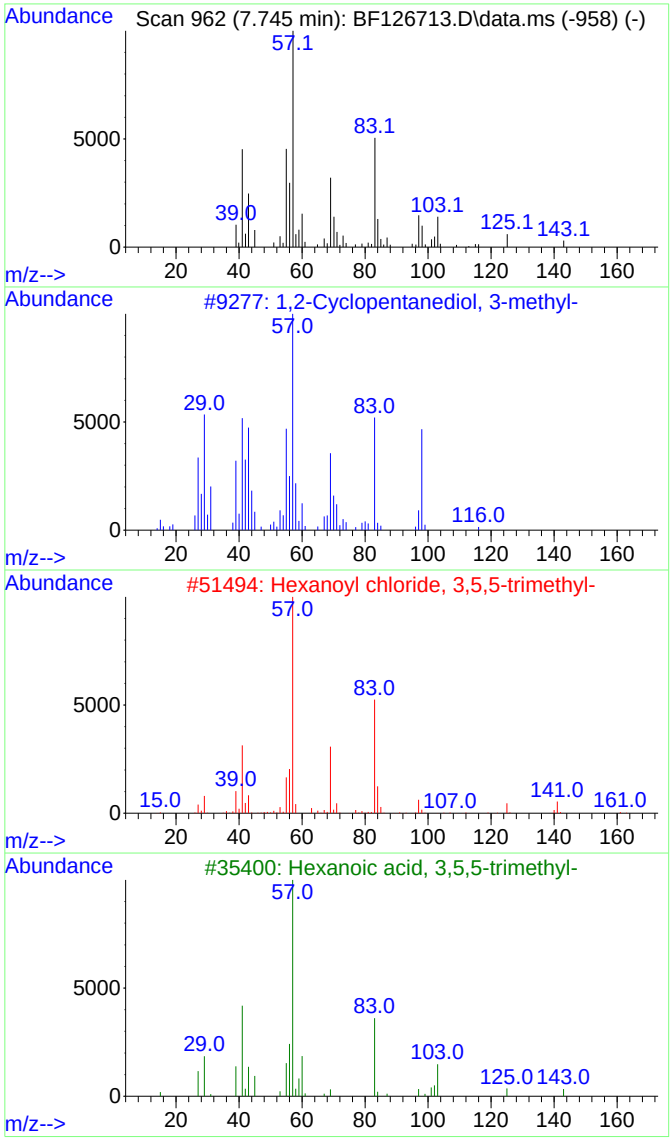
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

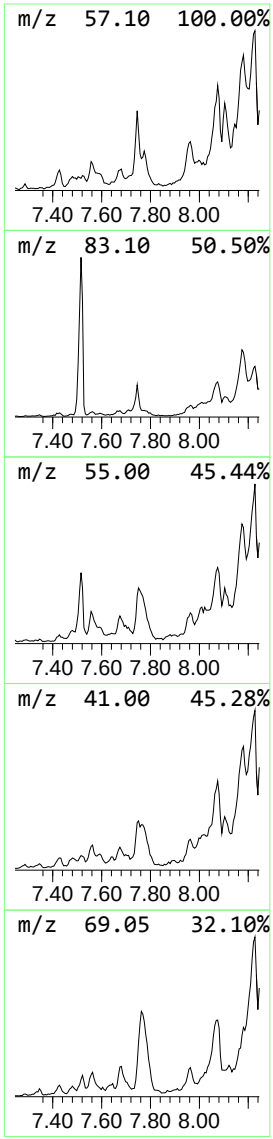
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2-Cyclopentanediol, 3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.745	3.33 ng	594641	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclopentanediol, 3-methyl-	116	C6H12O2	027583-37-5	58
2	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	53
3	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	50
4	Octyl angelate, 2-	212	C13H24O2	1000383-59-9	38
5	Propanoic acid, 2,2-dimethyl-, c...	184	C11H20O2	029878-49-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

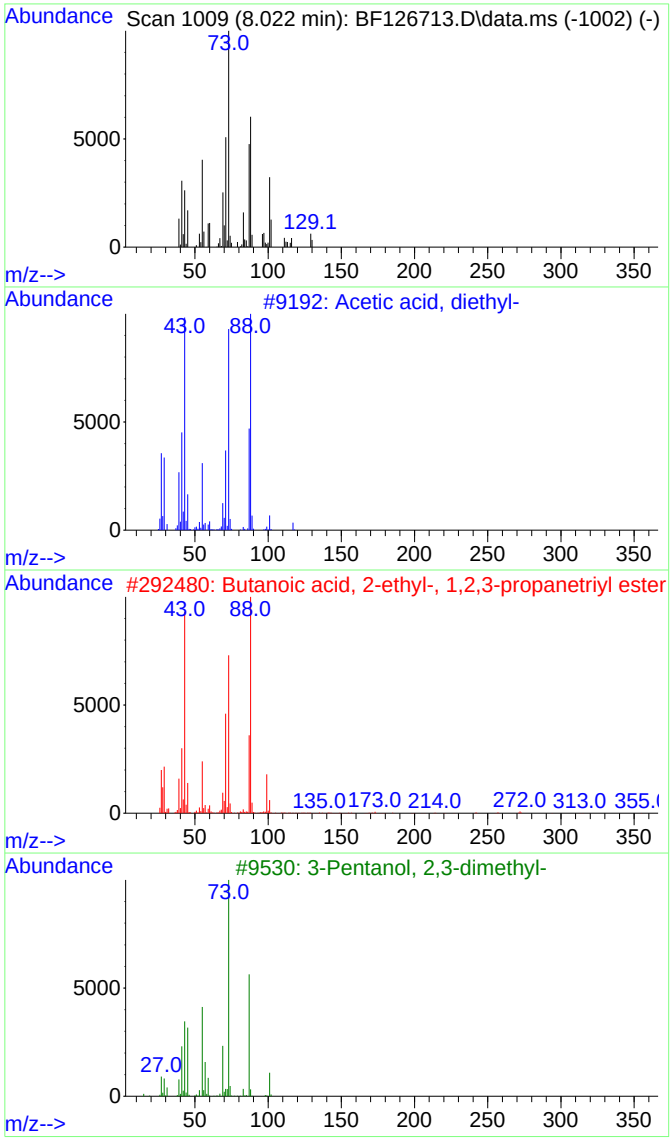
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

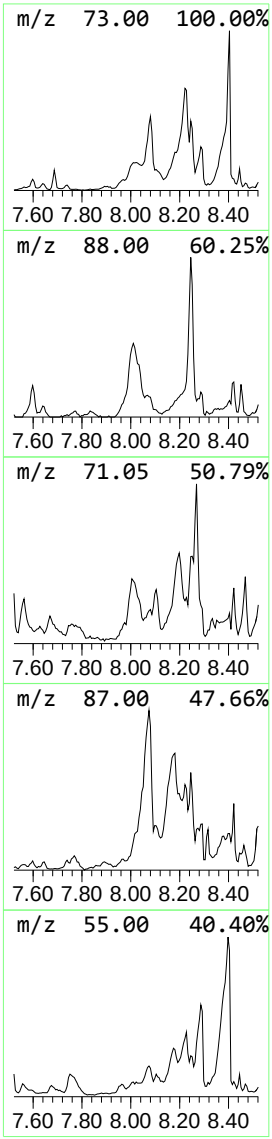
****

Peak Number 4 unknown8.022 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	2.58 ng	460860	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	47
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	43
3	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	27
4	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25
5	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

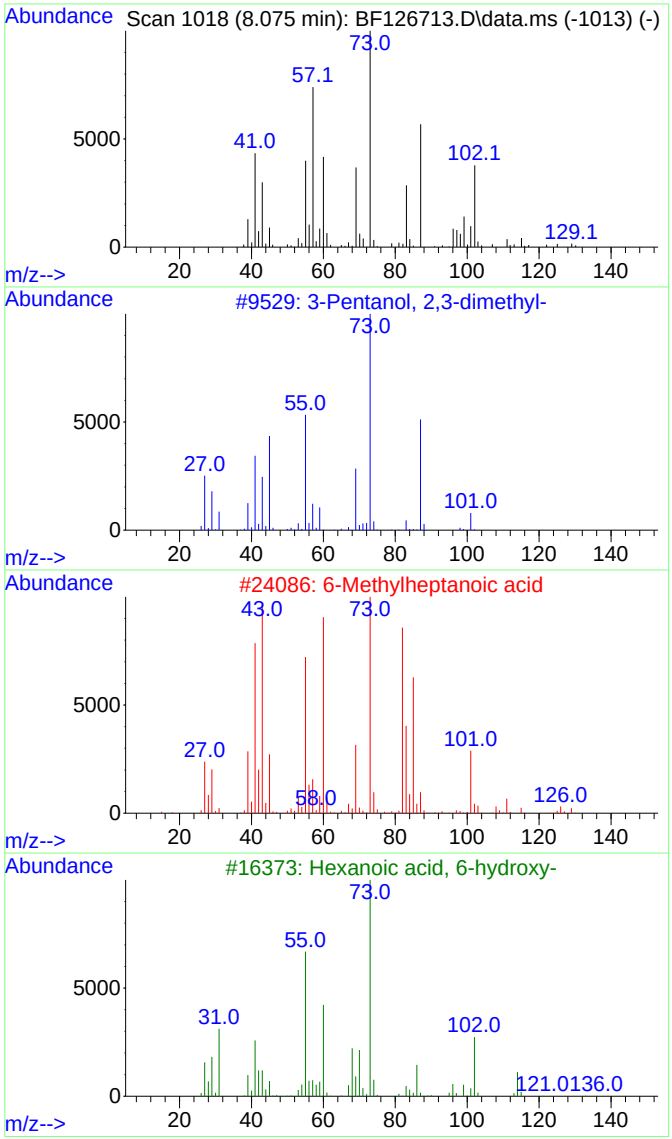
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

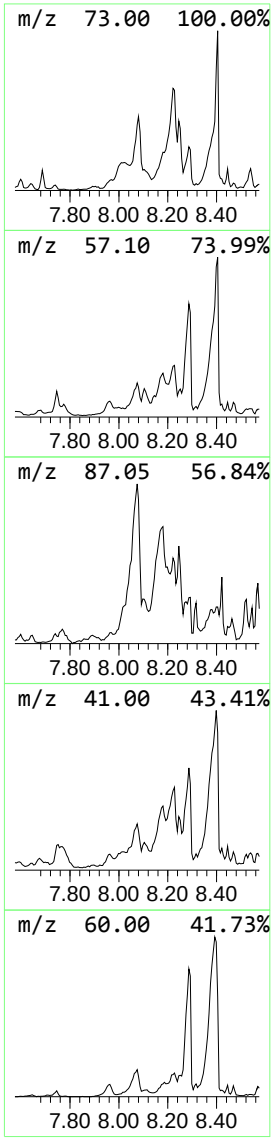
****

Peak Number 5 unknown8.075 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	5.73 ng	1023050	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	35
2	6-Methylheptanoic acid	144	C8H16O2	000929-10-2	25
3	Hexanoic acid, 6-hydroxy-	132	C6H12O3	001191-25-9	16
4	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	14
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

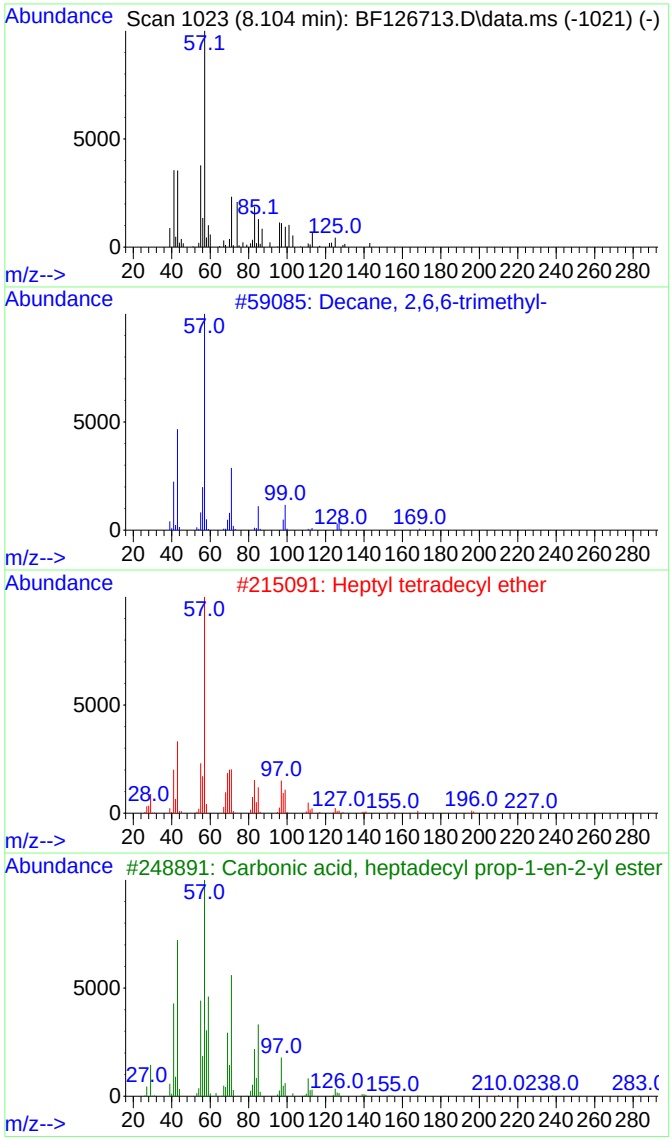
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

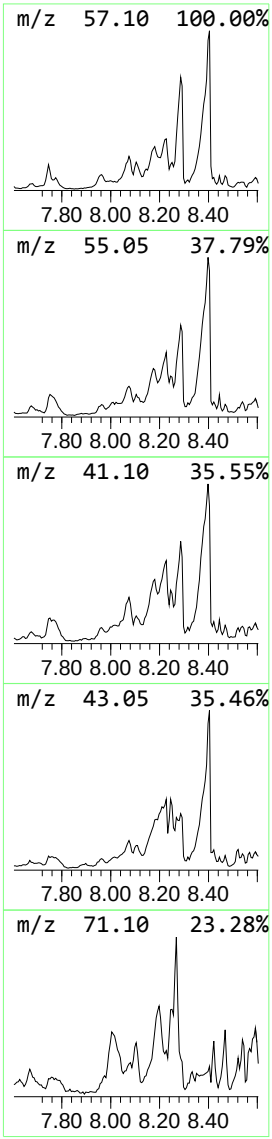
****

Peak Number 6 unknown8.104 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	2.72 ng	485546	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	35
2	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	32
3	Carbonic acid, heptadecyl prop-1...	340	C21H40O3	1000382-90-2	32
4	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	27
5	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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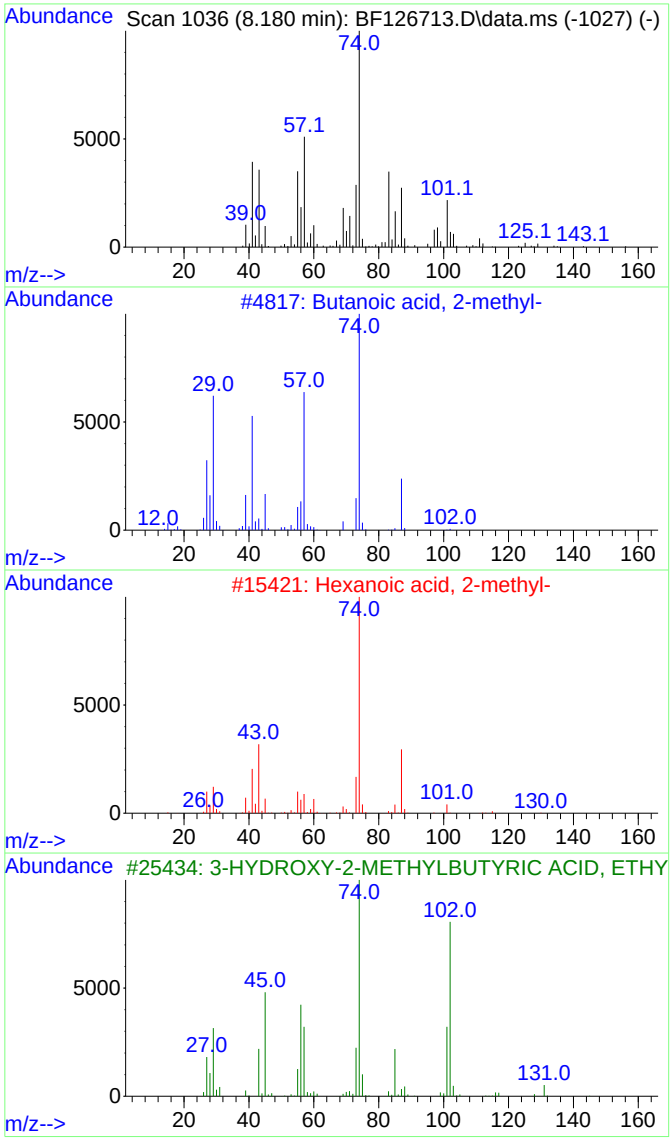
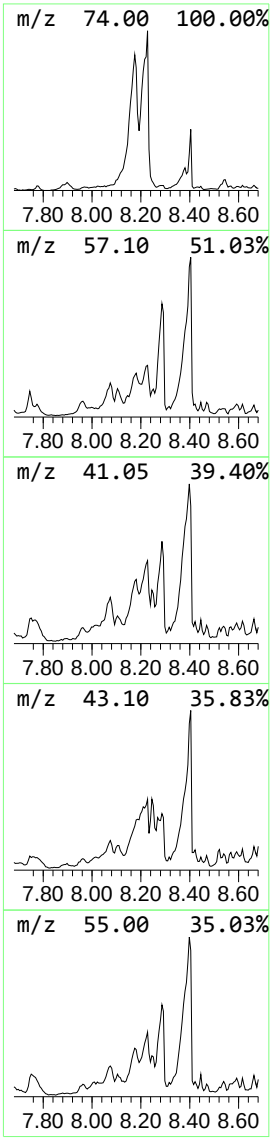
Peak Number 7 unknown8.180 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.180	10.20 ng	1819840	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	37
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	28
3	3-HYDROXY-2-METHYLBUTYRIC ACID, ...	146	C7H14O3	027372-03-8	28
4	Succinamic acid	117	C4H7NO3	000638-32-4	28
5	Hexanoic acid, 5-methyl-, methyl...	144	C8H16O2	002177-83-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

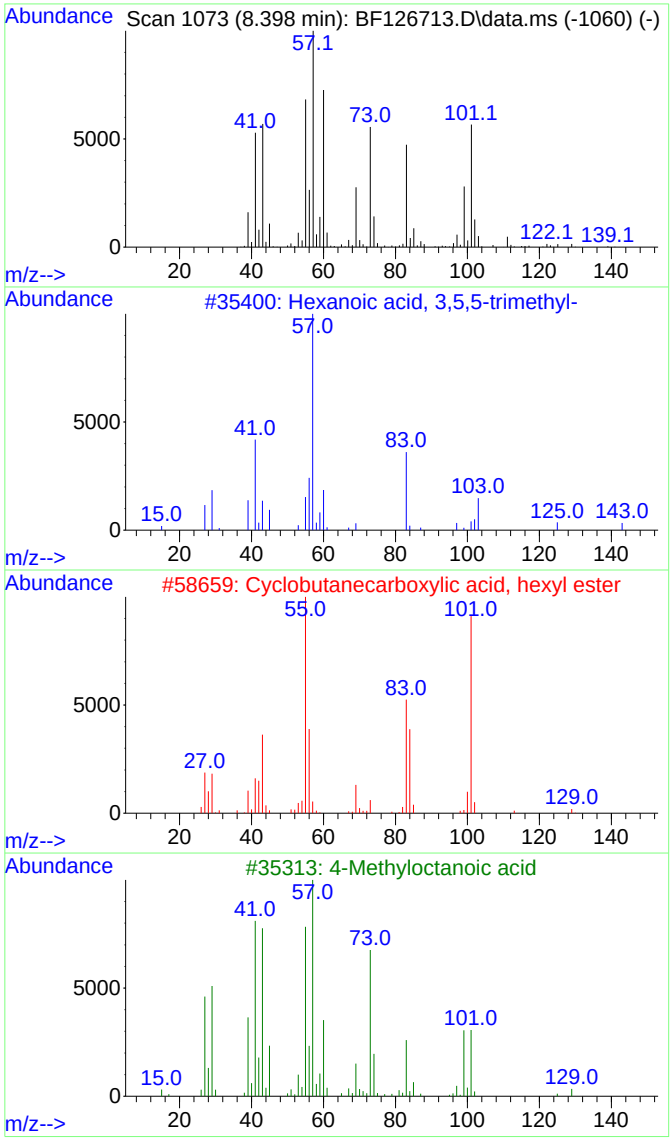
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

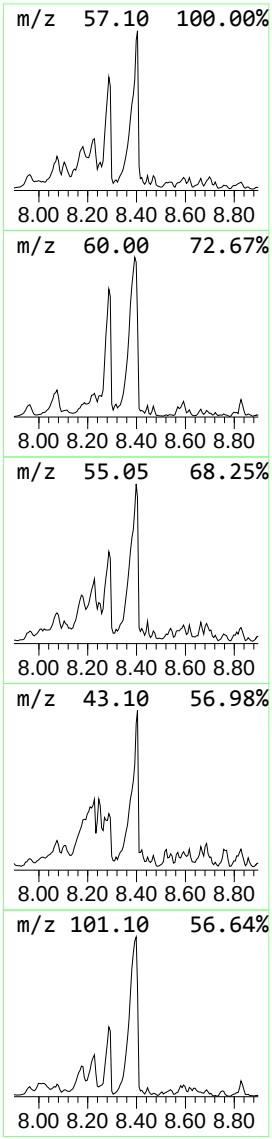
****

Peak Number 8 unknown8.398 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.398	24.10 ng	4301290	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	38
2	Cyclobutanecarboxylic acid, hexy...	184	C11H20O2	1000280-40-3	38
3	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	37
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	35
5	2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

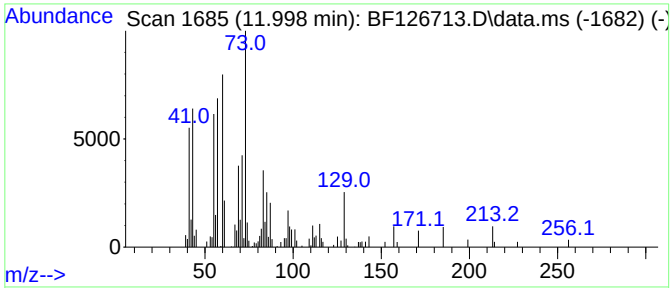
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

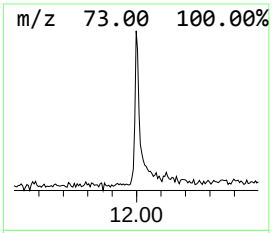
****

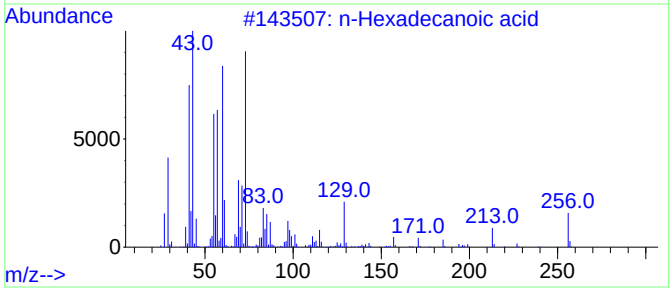
Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

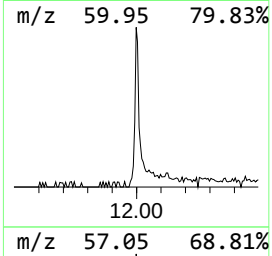
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.54 ng	173633	Phenanthrene-d10	11.486

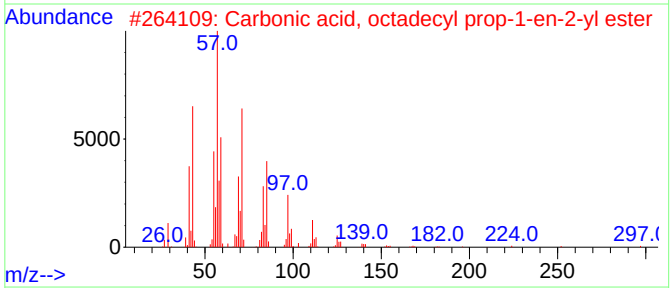
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15
3	Dodecane	170	C12H26	000112-40-3	11
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	11
5	Tridecane	184	C13H28	000629-50-5	11

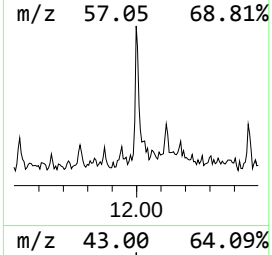


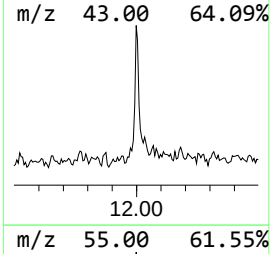


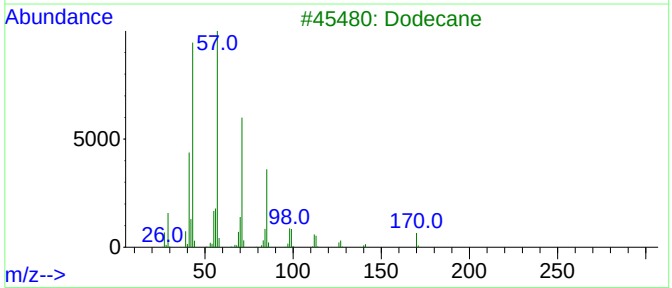


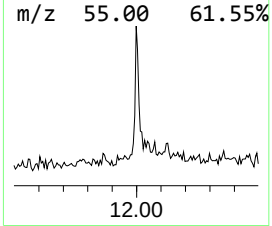












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012722\
Data File : BF126713.D
Acq On : 27 Jan 2022 18:36
Operator : CG/JU
Sample : N1301-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.281	32.0	ng	1805600	1	6.957	1129320	20.0
unknown7.039	7.039	3.2	ng	179095	1	6.957	1129320	20.0
1,2-Cyclopentan...	7.745	3.3	ng	594641	2	8.239	3569460	20.0
unknown8.022	8.022	2.6	ng	460860	2	8.239	3569460	20.0
unknown8.075	8.075	5.7	ng	1023050	2	8.239	3569460	20.0
unknown8.104	8.104	2.7	ng	485546	2	8.239	3569460	20.0
unknown8.180	8.180	10.2	ng	1819840	2	8.239	3569460	20.0
unknown8.398	8.398	24.1	ng	4301290	2	8.239	3569460	20.0
n-Hexadecanoic ...	11.998	2.5	ng	173633	4	11.486	1364790	20.0