LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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: BF125413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	15	rVB	241924	296054	23.02%	1.916%
2	3.957	314	318	324	rBV2	13770	17379	1.35%	0.112%
3	5.093	508	511	516	rBV	31584	34368	2.67%	0.222%
4	5.498	577	580	589	rBV	898901	828367	64.42%	5.362%
5	6.510	749	752	763	rBV	1020747	873026	67.90%	5.651%
6	6.881	812	815	819	rBV	1103979	1003649	78.06%	6.497%
7	7.416	900	906	907	rBV2	19596	23394	1.82%	0.151%
8	7.445	907	911	920	rVB	634103	564965	43.94%	3.657%
9	7.528	920	925	928	rVB5	19579	27942	2.17%	0.181%
10	7.569	928	932	935	rBV6	10134	16855	1.31%	0.109%
11	7.687	949	952	955	rVB2	17619	20734	1.61%	0.134%
12	7.804	970	972	976	rVB4	19446	19968	1.55%	0.129%
13	7.904	987	989	992	rBV3	14027	16021	1.25%	0.104%
14	8.069	1014	1017	1020	rBV4	27189	33954	2.64%	0.220%
15	8.169	1030	1034	1037	rBV	1472850	1247106	96.99%	8.073%
16	8.222	1040	1043	1045	rVB2	33913	34134	2.65%	0.221%
17	8.369	1065	1068	1070	rVB2	16908	16103	1.25%	0.104%
18	8.457	1079	1083	1086	rVB5	17924	22114	1.72%	0.143%
19	8.551	1094	1099	1101	rVB5	12522	17148	1.33%	0.111%
20	8.581	1101	1104	1106	rBV	43458	33567	2.61%	0.217%
21	8.669	1116	1119	1122	rBV3	20639	19275	1.50%	0.125%
22	8.751	1131	1133	1137	rBV2	43114	39395	3.06%	0.255%
23	8.828	1142	1146	1147	rBV4	11232	15349	1.19%	0.099%
24	8.939	1163	1165	1168	rBV3	12427	16144	1.26%	0.105%
25	8.986	1171	1173	1176	rVB3	30444	25138	1.96%	0.163%
26	9.110	1191	1194	1199	rBV5	20259	31406	2.44%	0.203%
27	9.181	1204	1206	1209	rBV	61533	51031	3.97%	0.330%
28	9.239	1212	1216	1221	rBV	1195405	990936	77.07%	6.415%
29	9.316	1226	1229	1233	rVB2	65518	63806	4.96%	0.413%
30	9.392	1239	1242	1244	rVB3	28593	27124	2.11%	0.176%
31	9.510	1258	1262	1264	rBV4	20590	25118	1.95%	0.163%
32	9.581	1271	1274	1276	rBV2	33541	34971	2.72%	0.226%
33	9.604	1276	1278	1280	rVB2	20550	17150	1.33%	0.111%
34	9.639	1280	1284	1286	rBV2	75610	82179	6.39%	0.532%
35	9.663	1286	1288	1291	rVV3	15911	15571	1.21%	0.101%
36	9.698	1291	1294	1299	rVB6	27302	30835	2.40%	0.200%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

37	9.786	1306	1309	1311	rBV2	30822	28923	2.25%	0.187%
38	9.845	1316	1319	1322	rVB	58927	52230	4.06%	0.338%
39	9.922	1327	1332	1336	rBV	1513509	1285816	100.00%	8.323%
40	9.951	1336	1337	1342	rVB4	24117	24142	1.88%	0.156%
41	10.028	1347	1350	1354	rBV5	24528	33237	2.58%	0.215%
42	10.086	1354	1360	1361	rBV5	16575	27563	2.14%	0.178%
43	10.110	1361	1364	1365	rBV2	16866	18552	1.44%	0.120%
44	10.163	1371	1373	1377	rBV4	40558	44248	3.44%	0.286%
45	10.239	1383	1386	1389	rBV3	33510	43902	3.41%	0.284%
46	10.345	1397	1404	1407	rBV2	89427	95986	7.46%	0.621%
47	10.463	1421	1424	1426	rBV4	12568	16817	1.31%	0.109%
48	10.563	1438	1441	1447	rVB	70401	96996	7.54%	0.628%
49	10.616	1447	1450	1454	rBV6	20092	21849	1.70%	0.141%
50	10.710	1463	1466	1471	rVB	353865	292486	22.75%	1.893%
51	10.833	1482	1487	1490	rBV	136794	171065	13.30%	1.107%
52	11.010	1515	1517	1520	rBV3	17293	18764	1.46%	0.121%
53	11.145	1537	1540	1542	rBV4	13924	18195	1.42%	0.118%
54	11.269	1558	1561	1563	rBV	63245	53259	4.14%	0.345%
55	11.298	1563	1566	1572	rVB2	98377	112231	8.73%	0.727%
56	11.410	1582	1585	1588	rBV	1308857	1158173	90.07%	7.497%
57	11.433	1588	1589	1591	rVV	114795	79424	6.18%	0.514%
58	11.457	1591	1593	1596	rVV4	37400	42735	3.32%	0.277%
59	11.486	1596	1598	1601	rVB	27658	21373	1.66%	0.138%
60	11.645	1622	1625	1627	rBV3	36826	35515	2.76%	0.230%
61	11.698	1631	1634	1637	rVV	51804	51940	4.04%	0.336%
62	11.745	1639	1642	1647	rVB3	25733	39365	3.06%	0.255%
63	11.822	1653	1655	1659	rBV4	12642	17852	1.39%	0.116%
64	11.927	1668	1673	1679	rBV2	81342	150658	11.72%	0.975%
65	12.022	1686	1689	1692	rBV3	40393	40371	3.14%	0.261%
66	12.104	1700	1703	1706	rBV2	53208	48383	3.76%	0.313%
67	12.210	1718	1721	1723	rBV2	28066	28035	2.18%	0.181%
68	12.339	1741	1743	1745	rBV2	31042	26928	2.09%	0.174%
69	12.386	1748	1751	1753	rBV2	39318	34884	2.71%	0.226%
70	12.463	1761	1764	1766	rBV	57368	57113	4.44%	0.370%
71	12.492	1766	1769	1772	rVB2	74478	70974	5.52%	0.459%
72	12.627	1789	1792	1797	rBV	195459	196215	15.26%	1.270%
73	12.722	1805	1808	1812	rBV6	31368	52384	4.07%	0.339%
74	12.780	1816	1818	1820	rVB3	38168	29370	2.28%	0.190%
75	12.857	1825	1831	1836	rBV2	232570	307902	23.95%	1.993%
76	12.992	1851	1854	1863	rVB	902468	852975	66.34%	5.522%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

77	13.180	1884	1886	1889	rVB2	53819	45532	3.54%	0.295%
78	13.222	1890	1893	1896	rBV2	70952	76524	5.95%	0.495%
79	13.563	1949	1951	1956	rVB	88529	76420	5.94%	0.495%
80	13.892	2005	2007	2010	rBV2	115334	87343	6.79%	0.565%
81	14.057	2031	2035	2038	rBV	990640	974903	75.82%	6.311%
82	14.210	2058	2061	2066	rBV	178015	183317	14.26%	1.187%
83	14.516	2110	2113	2116	rVB	200248	164352	12.78%	1.064%
84	14.827	2164	2166	2169	rVB	155752	126268	9.82%	0.817%
85	15.174	2222	2225	2230	rVB	201568	241438	18.78%	1.563%
86	15.551	2285	2289	2297	rVB3	686296	1040965	80.96%	6.738%

Sum of corrected areas: 15448168

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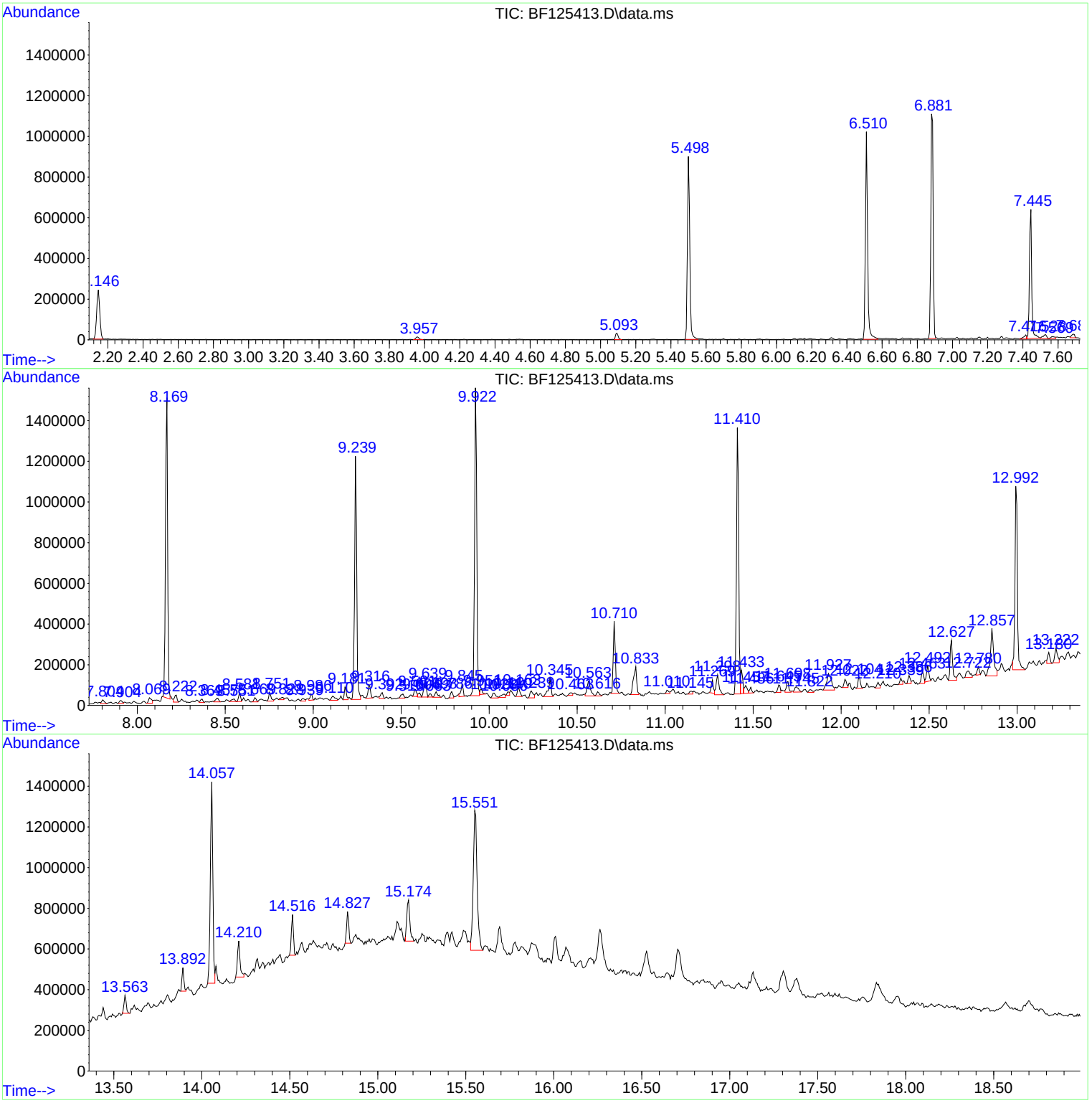
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-SF-02-006-A

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

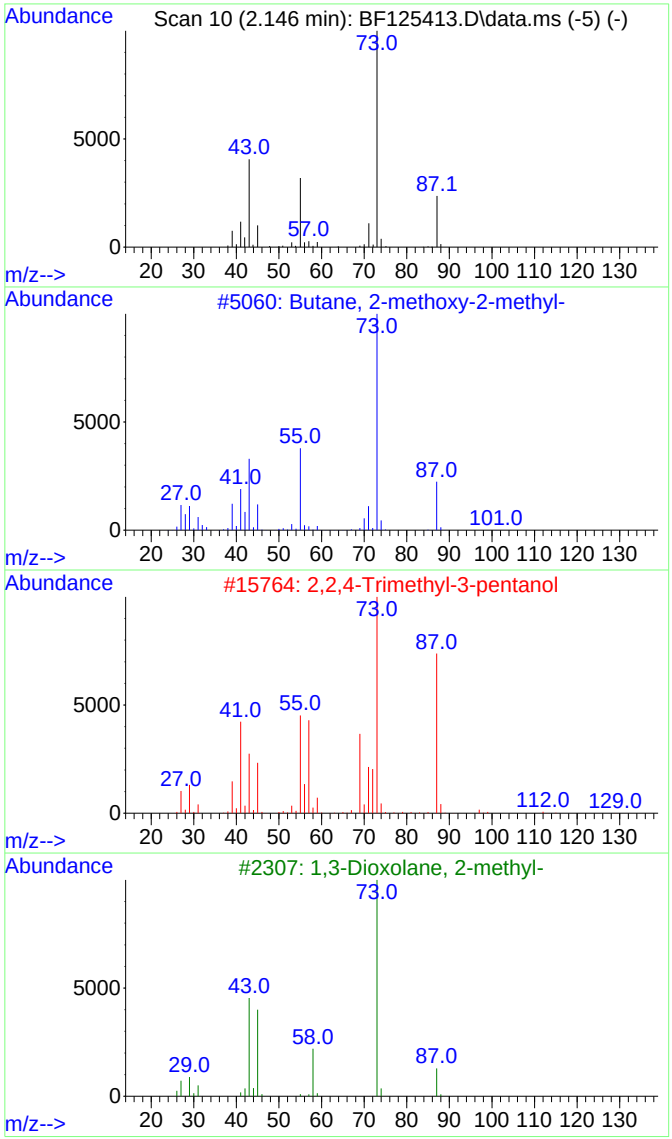
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

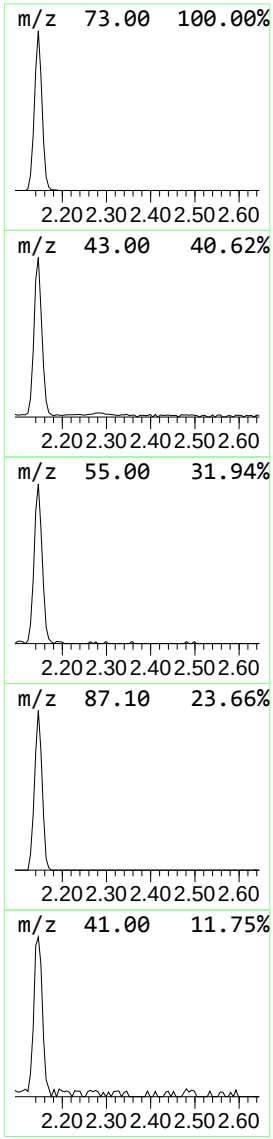
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	5.90 ng	296054	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

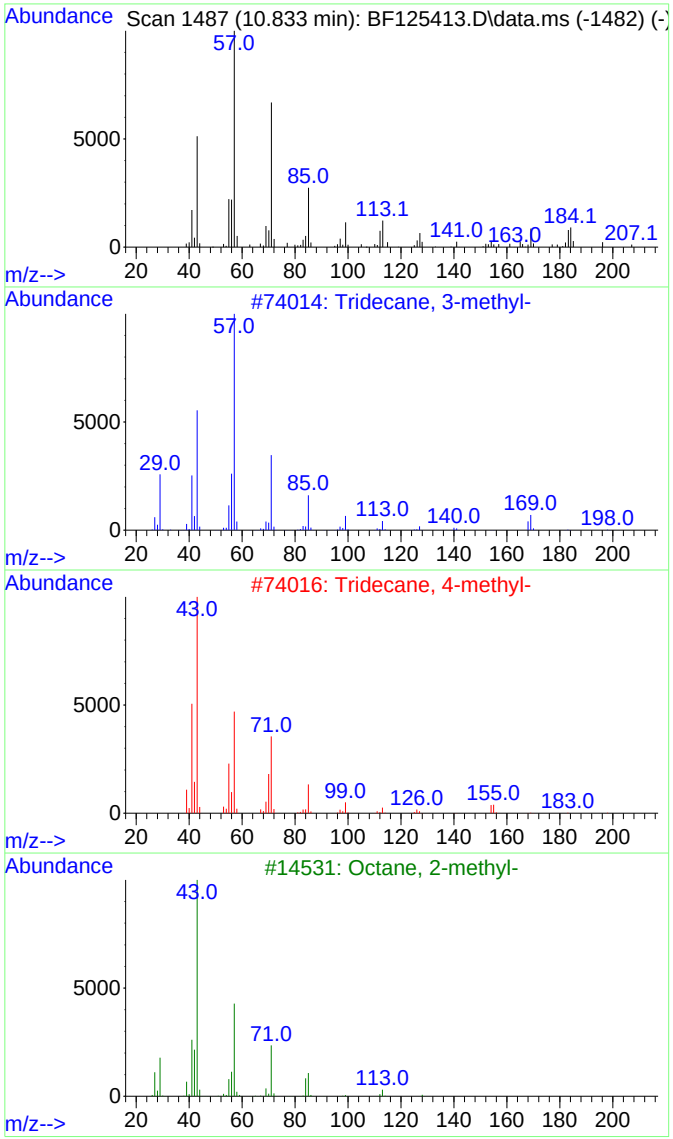
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

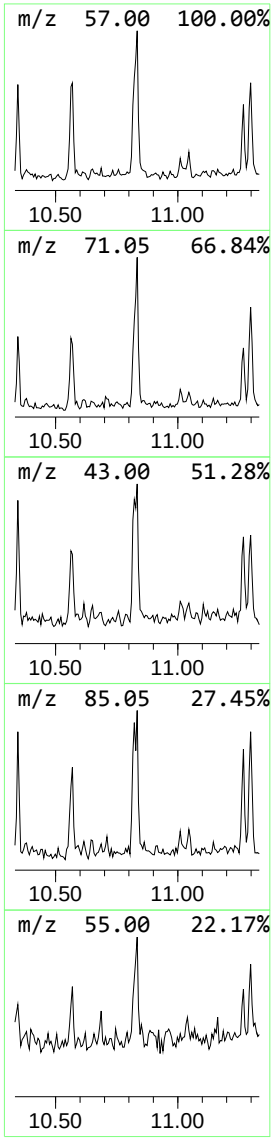
****

Peak Number 2 Tridecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	2.95 ng	171065	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
2	Tridecane, 4-methyl-	198	C14H30	026730-12-1	64
3	Octane, 2-methyl-	128	C9H20	003221-61-2	64
4	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	58
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

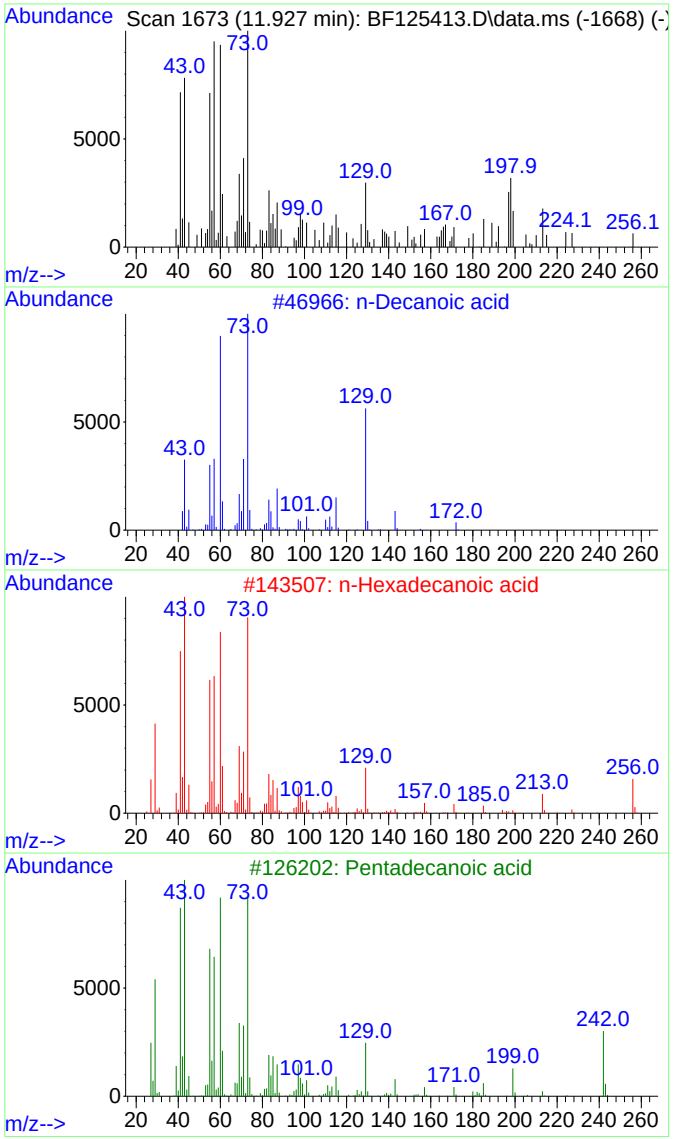
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

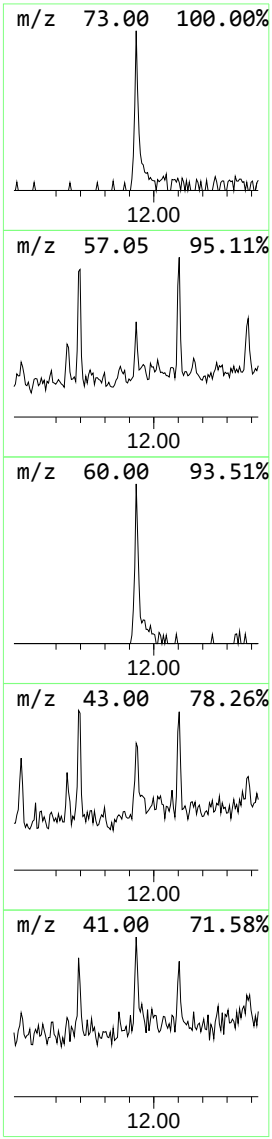
****

Peak Number 3 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	2.60 ng	150658	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	59
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





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Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-SF-02-006-A

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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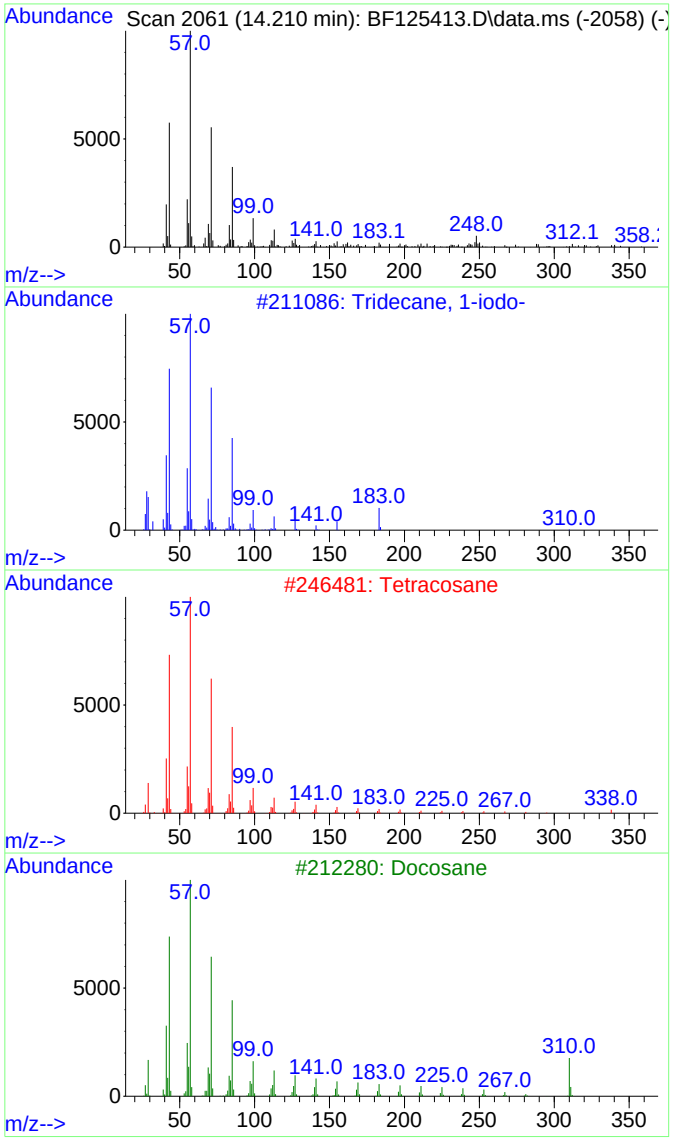
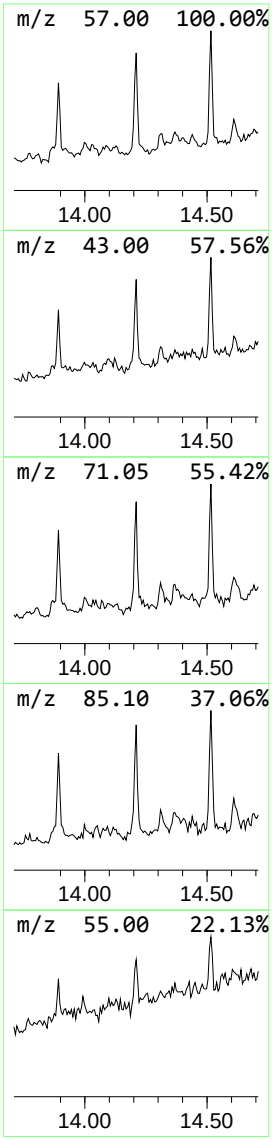
Peak Number 4 Tridecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	3.76 ng	183317	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Docosane	310	C22H46	000629-97-0	81
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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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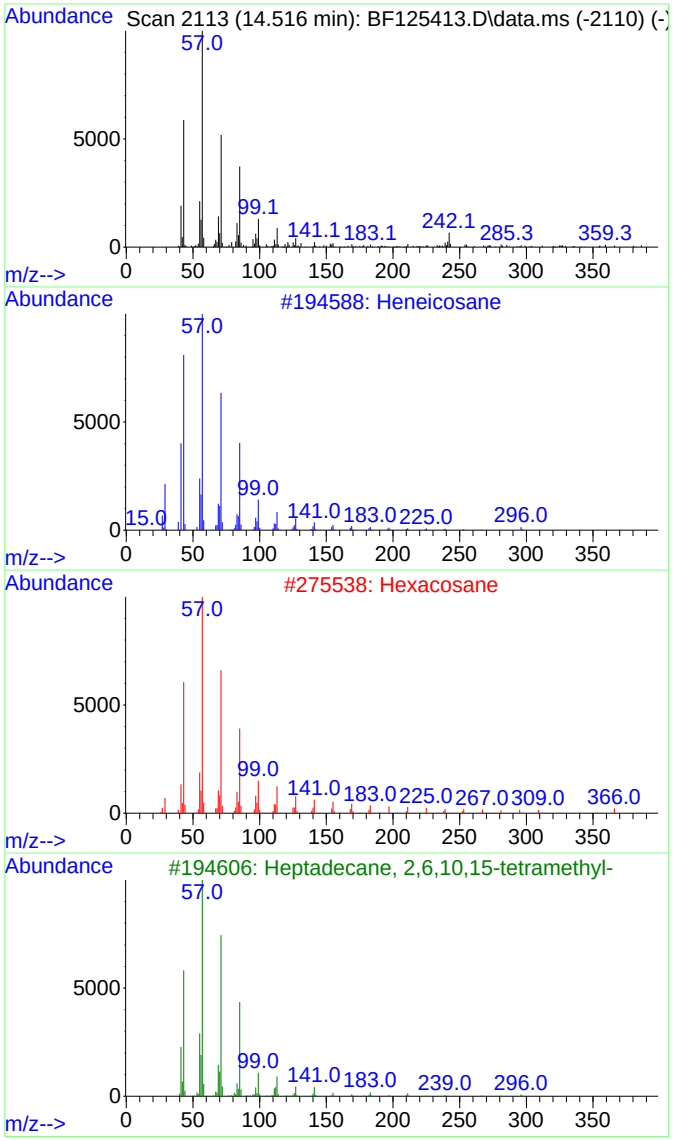
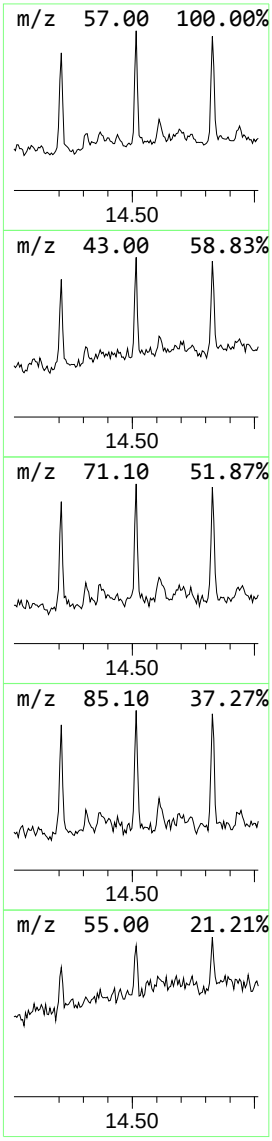
Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	3.37 ng	164352	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
4	Tetradecane, 6,9-dimethyl-	226	C16H34	055045-13-1	87
5	Tricosane	324	C23H48	000638-67-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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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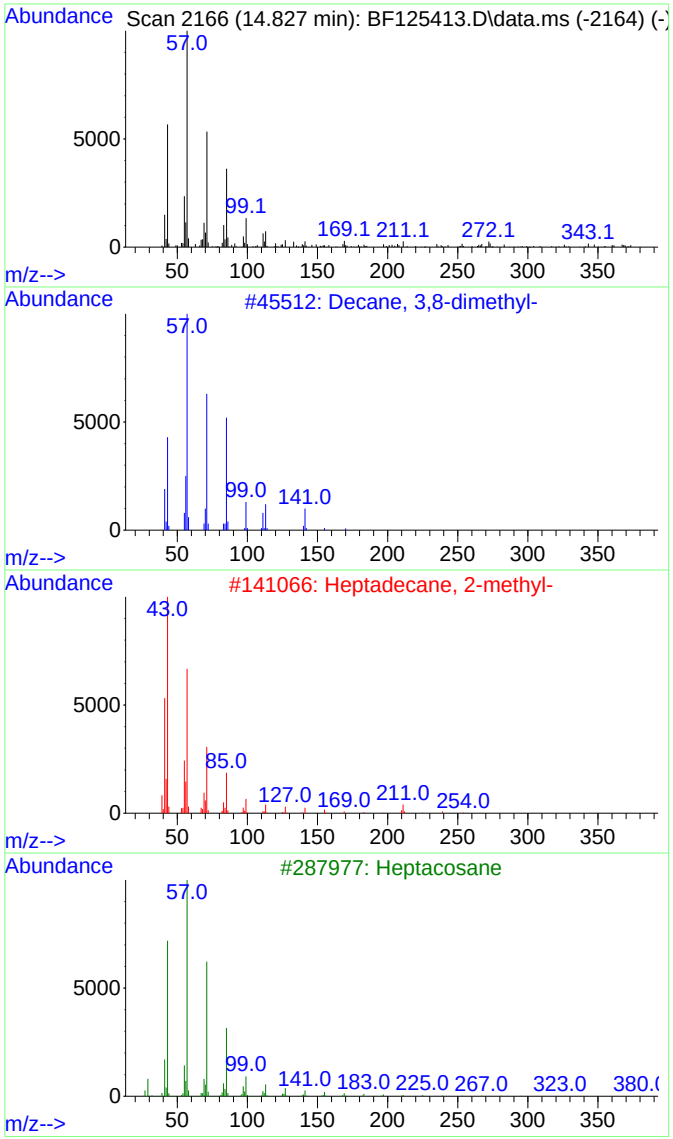
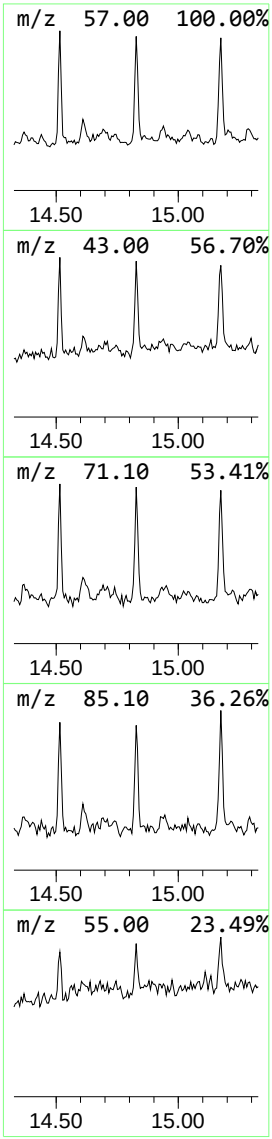
Peak Number 6 Decane, 3,8-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	2.43 ng	126268	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	83
5	Undecane, 3-methyl-	170	C12H26	001002-43-3	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

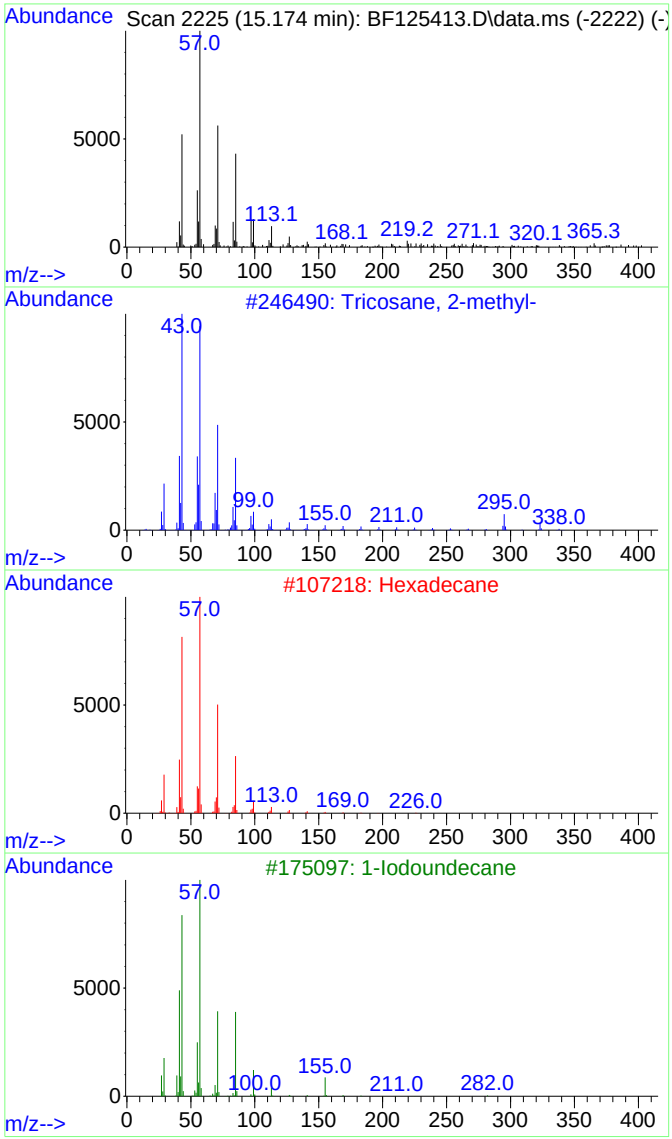
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

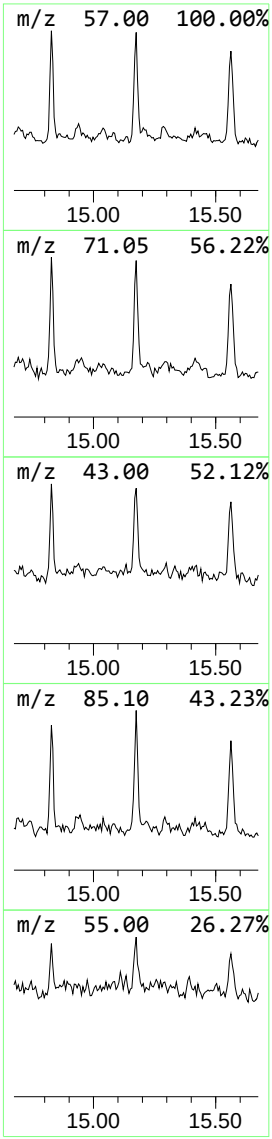
****

Peak Number 7 Tricosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	4.64 ng	241438	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
2	Hexadecane	226	C16H34	000544-76-3	83
3	1-Iodoundecane	282	C11H23I	004282-44-4	81
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125413.D
Acq On : 9 Sep 2021 15:24
Operator : JU/CG
Sample : M3680-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-02-006-A

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	5.9	ng	296054	1	6.887	1003650	20.0
Tridecane, 3-me...	10.833	3.0	ng	171065	4	11.410	1158170	20.0
n-Decanoic acid	11.928	2.6	ng	150658	4	11.410	1158170	20.0
Tridecane, 1-iodo-	14.210	3.8	ng	183317	5	14.057	974903	20.0
Heneicosane	14.515	3.4	ng	164352	5	14.057	974903	20.0
Decane, 3,8-dim...	14.827	2.4	ng	126268	6	15.551	1040970	20.0
Tricosane, 2-me...	15.174	4.6	ng	241438	6	15.551	1040970	20.0