LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125753.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	23	rVB	1270014	1614692	36.66%	4.295%
2	2.293	31	35	41	rVB	57063	73814	1.68%	0.196%
3	5.110	504	514	520	rBV	39562	56511	1.28%	0.150%
4	5.504	576	581	584	rBV	3547935	3432853	77.93%	9.131%
5	6.504	746	751	754	rBV	3249051	3382084	76.78%	8.996%
6	6.887	812	816	819	rBV	1550656	1165054	26.45%	3.099%
7	7.445	906	911	914	rBV	2544037	2218272	50.36%	5.900%
8	8.069	1013	1017	1027	rBV	131795	158331	3.59%	0.421%
9	8.169	1030	1034	1037	rBV	1911489	1595461	36.22%	4.244%
10	8.881	1152	1155	1158	rBV	83841	66494	1.51%	0.177%
11	9.245	1212	1217	1220	rBV	4723347	4405011	100.00%	11.716%
12	9.357	1233	1236	1240	rBV2	58131	62178	1.41%	0.165%
13	9.563	1267	1271	1272	rBV3	42578	53077	1.20%	0.141%
14	9.581	1272	1274	1276	rVV	96090	80745	1.83%	0.215%
15	9.604	1276	1278	1281	rVB3	58562	54881	1.25%	0.146%
16	9.645	1281	1285	1287	rBV2	114894	158271	3.59%	0.421%
17	9.698	1291	1294	1297	rVV4	61456	71697	1.63%	0.191%
18	9.798	1307	1311	1313	rBV4	103739	138931	3.15%	0.370%
19	9.839	1315	1318	1320	rVB	146709	147140	3.34%	0.391%
20	9.922	1325	1332	1336	rBV	2218327	2103977	47.76%	5.596%
21	9.963	1337	1339	1341	rBV2	82850	68831	1.56%	0.183%
22	10.180	1374	1376	1379	rBV3	106601	123648	2.81%	0.329%
23	10.210	1379	1381	1383	rVB2	98549	68149	1.55%	0.181%
24	10.239	1384	1386	1388	rBV2	131742	131985	3.00%	0.351%
25	10.298	1393	1396	1399	rBV5	147687	187788	4.26%	0.499%
26	10.333	1399	1402	1404	rBV2	331389	312207	7.09%	0.830%
27	10.386	1409	1411	1413	rBV	229971	209430	4.75%	0.557%
28	10.575	1439	1443	1446	rBV	500821	672928	15.28%	1.790%
29	10.710	1462	1466	1469	rBV	2422873	2230558	50.64%	5.933%
30	10.845	1486	1489	1495	rBV	1255068	1312988	29.81%	3.492%
31	11.310	1565	1568	1575	rVB	1419947	1607086	36.48%	4.274%
32	11.410	1582	1585	1588	rBV	1716974	1575740	35.77%	4.191%
33	12.992	1851	1854	1863	rVB	3583544	3716274	84.36%	9.884%
34	14.045	2029	2033	2042	rVB	1268600	1215726	27.60%	3.234%
35	14.898	2176	2178	2183	rVB2	48511	51731	1.17%	0.138%
36	15.521	2278	2284	2294	rVB	986332	1320207	29.97%	3.511%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.239	2381	2406	2432	rBV5	230197	1752593	39.79%	4.661%

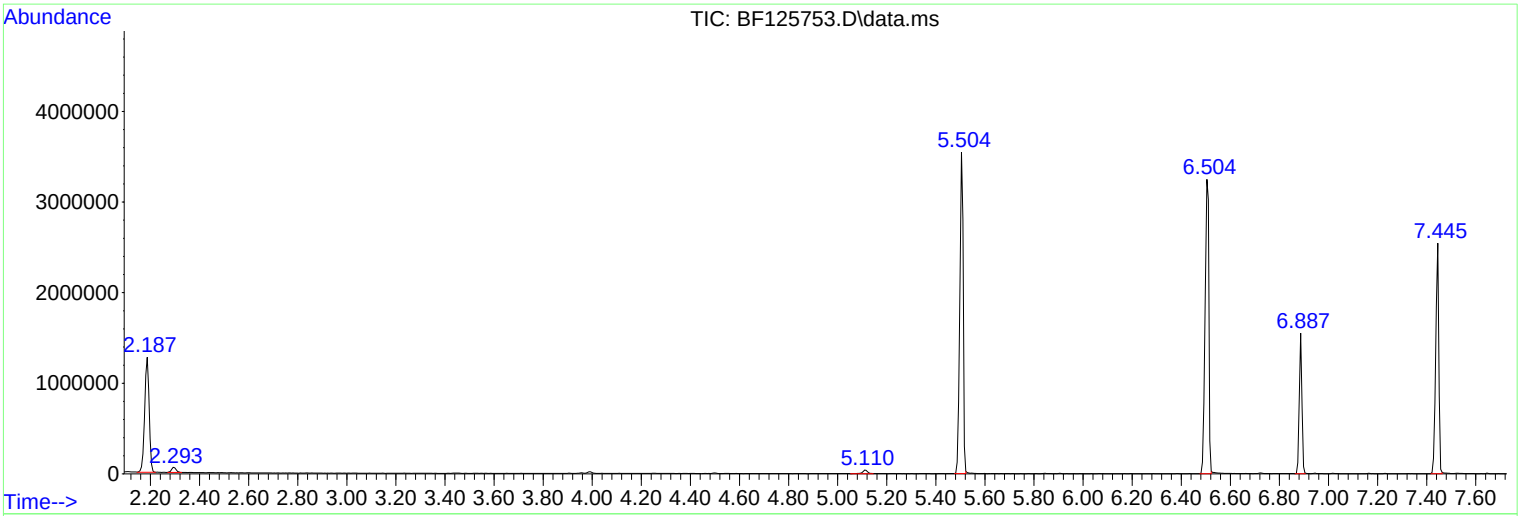
Sum of corrected areas: 37597343

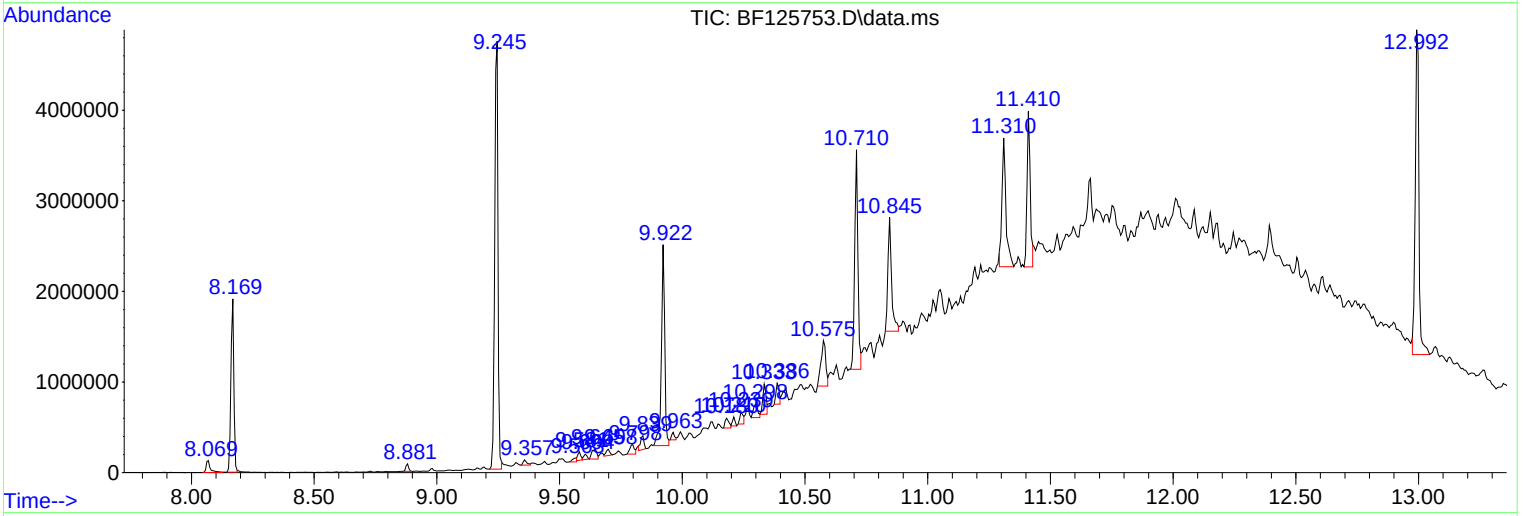
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

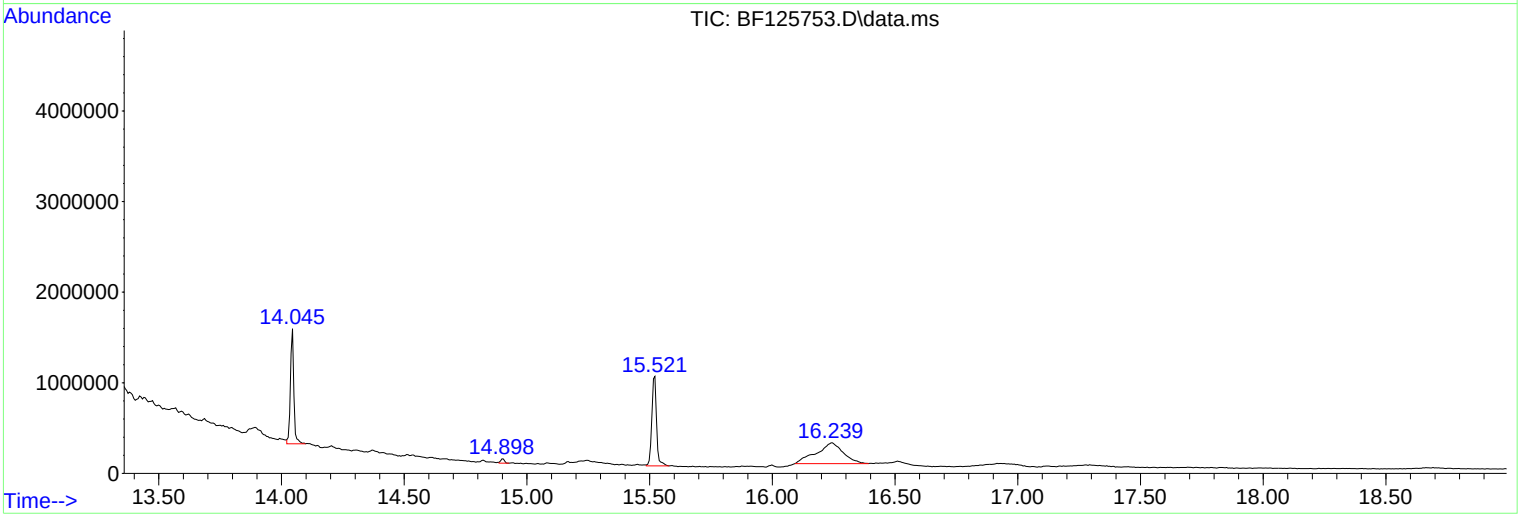
Instrument :
BNA_F
ClientSampleId :
26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

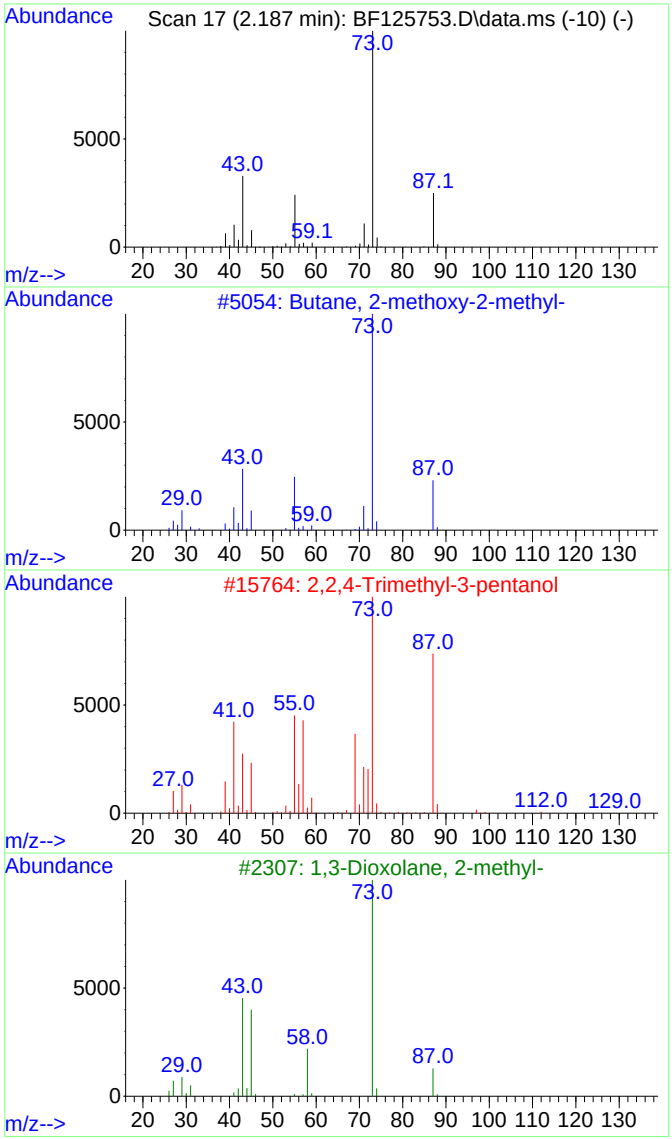
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

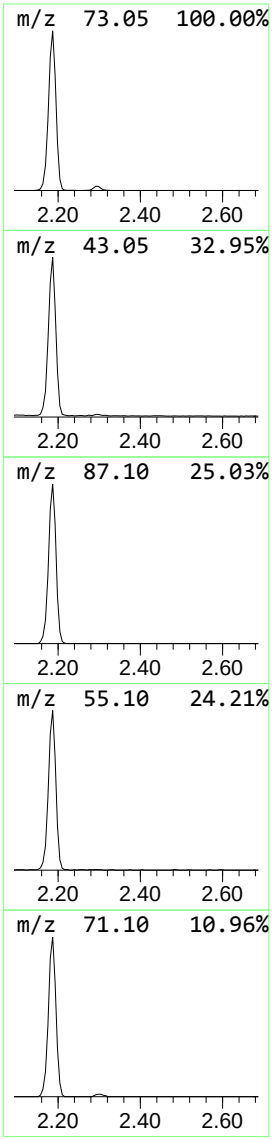
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	27.72 ng	1614690	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	83
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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

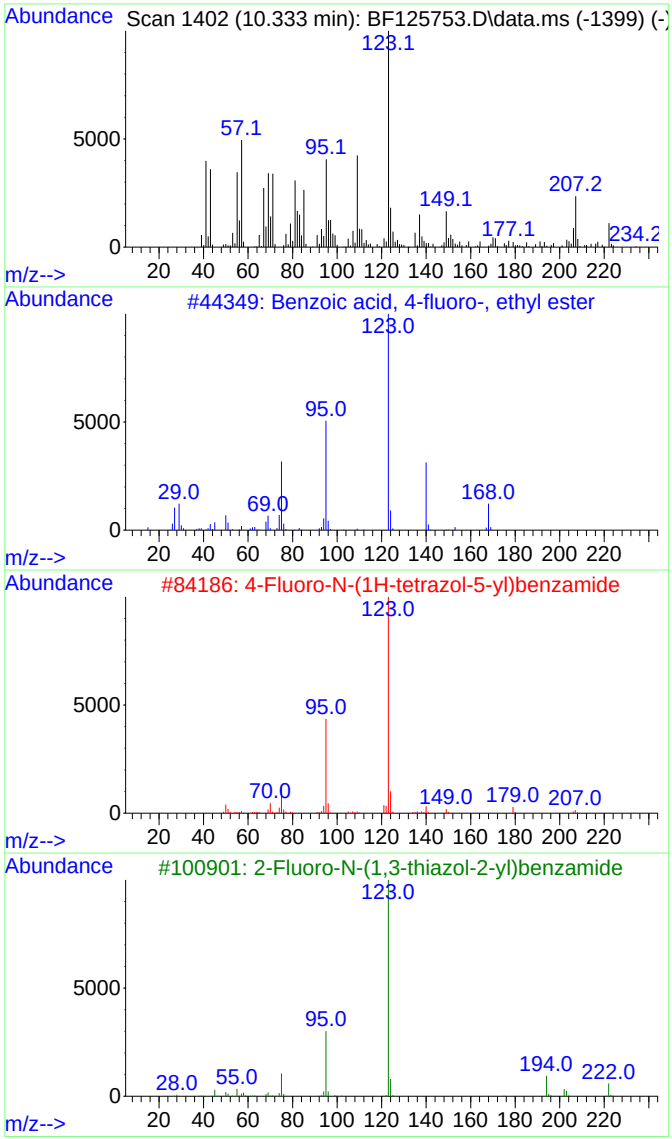
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

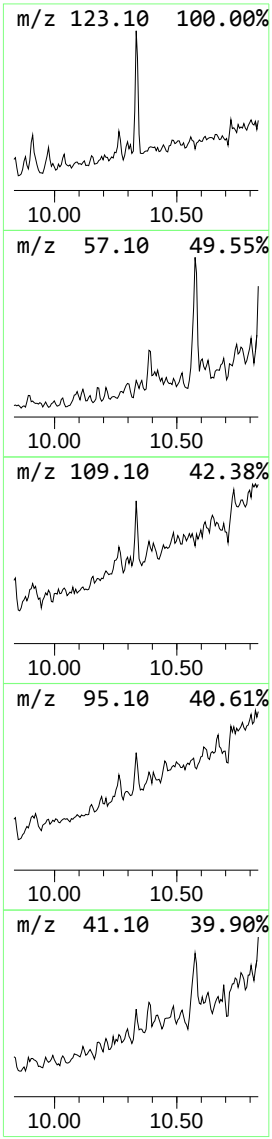
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzoic acid, 4-fluoro-, et... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.333	2.97 ng	312207	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-fluoro-, ethyl e...	168	C9H9FO2	000451-46-7	43
2	4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	43
3	2-Fluoro-N-(1,3-thiazol-2-yl)ben...	222	C10H7FN2OS	000319-38-0	43
4	Bromo-4-fluoroacetophenone	216	C8H6BrFO	000403-29-2	43
5	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

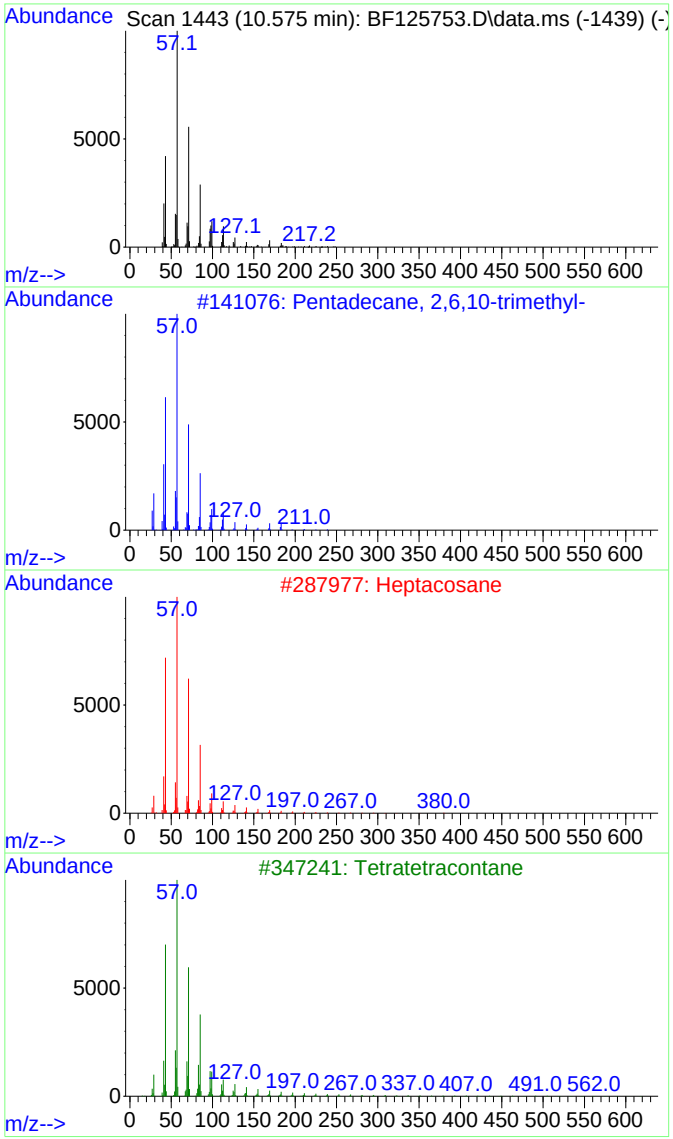
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

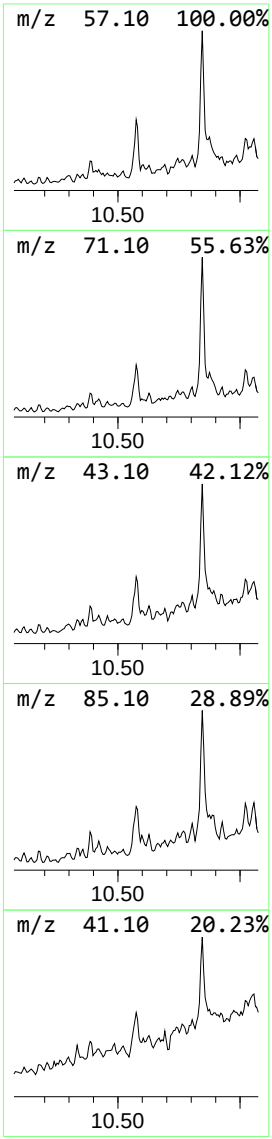
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	6.40 ng	672928	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
5	Eicosane	282	C20H42	000112-95-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

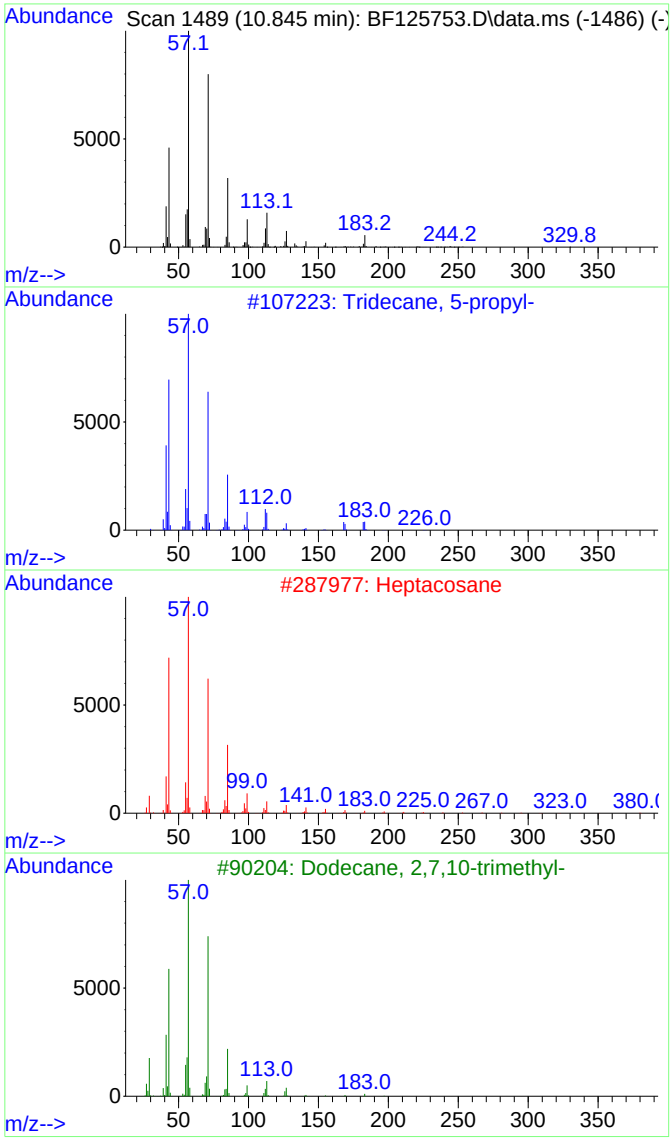
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

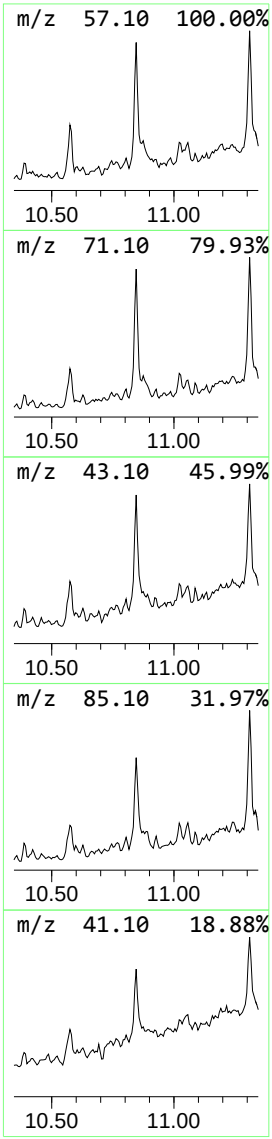
****

Peak Number 4 Tridecane, 5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	16.66 ng	1312990	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	93
2	Heptacosane	380	C27H56	000593-49-7	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	83
5	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

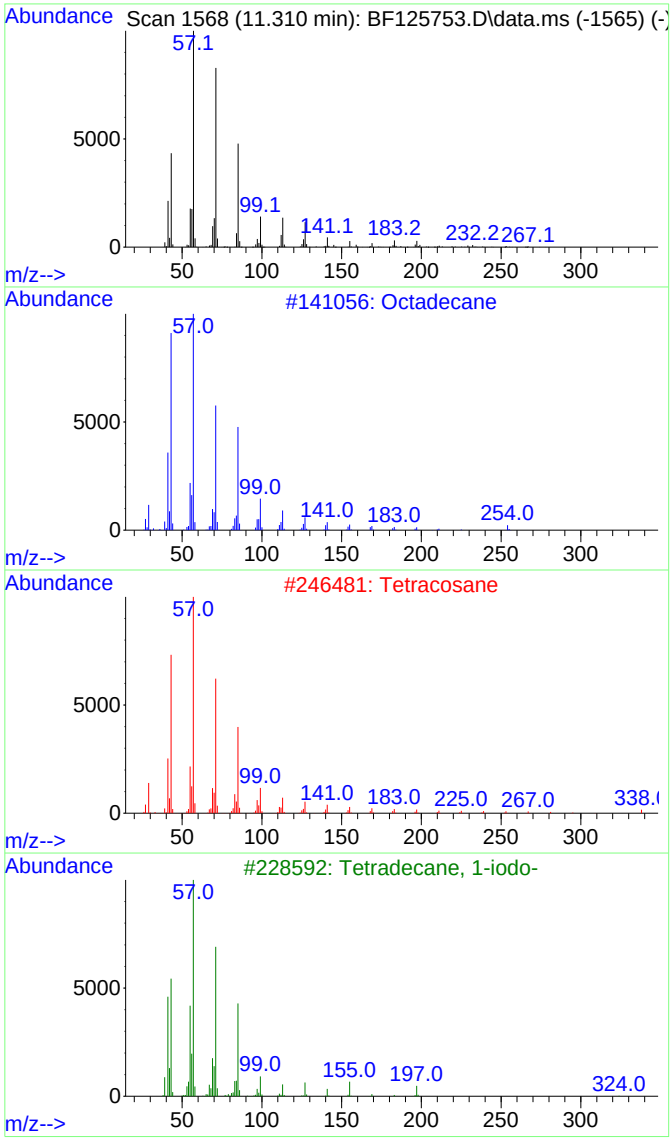
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

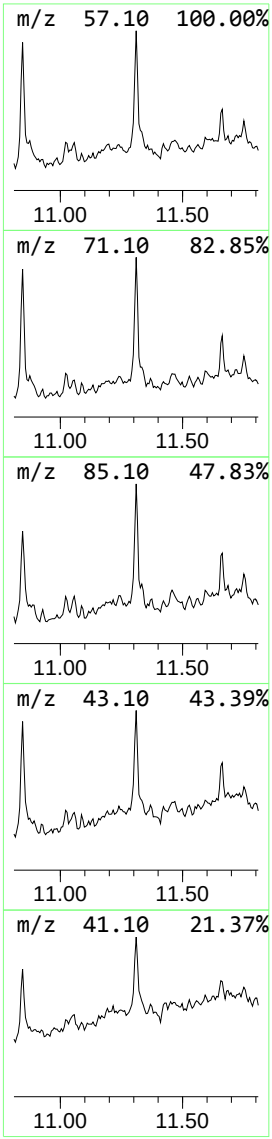
****

Peak Number 5 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.310	20.40 ng	1607090	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

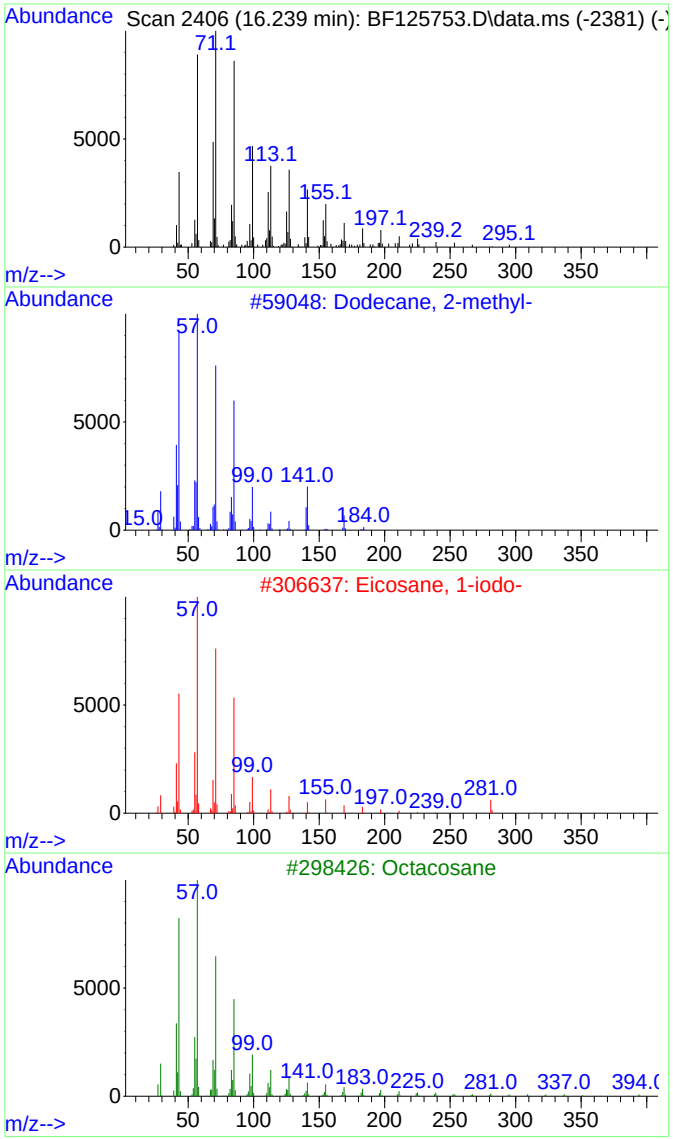
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

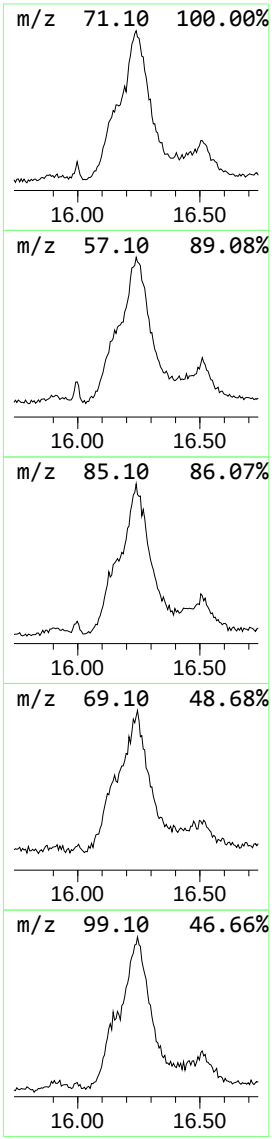
****

Peak Number 6 Dodecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.239	26.55 ng	1752590	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	62
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	59
3	Octacosane	394	C28H58	000630-02-4	53
4	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	50
5	Heptadecane	240	C17H36	000629-78-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125753.D
Acq On : 1 Oct 2021 15:36
Operator : JU/CG
Sample : M3999-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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...	2.187	27.7	ng	1614690	1	6.887	1165050	20.0
Benzoic acid, 4...	10.333	3.0	ng	312207	3	9.922	2103980	20.0
Pentadecane, 2,...	10.575	6.4	ng	672928	3	9.922	2103980	20.0
Tridecane, 5-pr...	10.845	16.7	ng	1312990	4	11.410	1575740	20.0
Octadecane	11.310	20.4	ng	1607090	4	11.410	1575740	20.0
Dodecane, 2-met...	16.239	26.6	ng	1752590	6	15.521	1320210	20.0