LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	21	rBV	9826	13510	1.11%	0.124%
2	5.028	496	500	505	rBV	29450	37601	3.09%	0.345%
3	5.422	563	567	583	rBV	1104006	1142293	93.78%	10.468%
4	6.422	733	737	752	rBV	1017176	1069815	87.83%	9.804%
5	6.793	796	800	807	rBV	336454	295841	24.29%	2.711%
6	7.351	891	895	899	rBV	747734	628104	51.57%	5.756%
7	7.387	899	901	905	rVV	44209	38203	3.14%	0.350%
8	7.434	905	909	912	rVB5	9059	13094	1.08%	0.120%
9	7.592	932	936	940	rVB5	14885	17670	1.45%	0.162%
10	8.069	1011	1017	1020	rBV	424268	390061	32.02%	3.575%
11	8.363	1062	1067	1070	rBV3	17701	26175	2.15%	0.240%
12	8.451	1079	1082	1085	rBV3	19247	15304	1.26%	0.140%
13	8.492	1085	1089	1091	rBV2	17386	15173	1.25%	0.139%
14	8.575	1099	1103	1106	rBV2	25083	25329	2.08%	0.232%
15	8.663	1115	1118	1121	rBV2	47488	40974	3.36%	0.375%
16	8.892	1153	1157	1159	rBV3	18124	15122	1.24%	0.139%
17	9.145	1196	1200	1203	rBV	1317353	1023694	84.05%	9.381%
18	9.228	1211	1214	1218	rBV	34229	30668	2.52%	0.281%
19	9.422	1241	1247	1251	rBV8	7859	15824	1.30%	0.145%
20	9.551	1264	1269	1271	rBV3	12885	15819	1.30%	0.145%
21	9.763	1302	1305	1309	rVB	29789	24063	1.98%	0.221%
22	9.822	1311	1315	1319	rBV	449178	349022	28.65%	3.198%
23	10.263	1387	1390	1392	rVB	33397	22797	1.87%	0.209%
24	10.486	1421	1428	1430	rBV	16014	19707	1.62%	0.181%
25	10.610	1445	1449	1459	rBV	782609	739332	60.70%	6.775%
26	10.739	1468	1471	1476	rBV	35869	45474	3.73%	0.417%
27	11.186	1545	1547	1550	rBV	27110	24568	2.02%	0.225%
28	11.216	1550	1552	1556	rVB2	16199	16963	1.39%	0.155%
29	11.310	1565	1568	1572	rBV	376307	369003	30.30%	3.382%
30	11.616	1618	1620	1623	rBV	23713	21009	1.72%	0.193%
31	11.722	1634	1638	1641	rBV	262571	223405	18.34%	2.047%
32	11.857	1657	1661	1669	rBV4	67712	117396	9.64%	1.076%
33	12.027	1687	1690	1692	rBV	23053	19624	1.61%	0.180%
34	12.369	1745	1748	1751	rBV2	15056	17290	1.42%	0.158%
35	12.410	1751	1755	1757	rVV	1255345	1126236	92.46%	10.321%
36	12.433	1757	1759	1766	rVV	771568	675424	55.45%	6.190%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.516	1770	1773	1778	rVV2	132529	141849	11.65%	1.300%
38	12.569	1780	1782	1788	rVB7	11446	19415	1.59%	0.178%
39	12.651	1793	1796	1800	rBV6	16611	23341	1.92%	0.214%
40	12.757	1812	1814	1817	rVB	30126	26033	2.14%	0.239%
41	12.792	1818	1820	1822	rVV	18880	14919	1.22%	0.137%
42	12.822	1822	1825	1828	rVB5	12549	14199	1.17%	0.130%
43	12.910	1836	1840	1849	rBV	1239770	1218025	100.00%	11.162%
44	13.157	1879	1882	1886	rVB3	22130	23610	1.94%	0.216%
45	13.357	1914	1916	1920	rVB4	19300	19023	1.56%	0.174%
46	13.498	1938	1940	1943	rVB2	21699	16420	1.35%	0.150%
47	13.833	1994	1997	2001	rBV5	22872	23714	1.95%	0.217%
48	13.963	2015	2019	2027	rBV	338875	382713	31.42%	3.507%
49	14.457	2101	2103	2105	rVB2	33190	26650	2.19%	0.244%
50	15.121	2213	2216	2220	rVB	54623	64742	5.32%	0.593%
51	15.445	2267	2271	2275	rBV	184515	215836	17.72%	1.978%

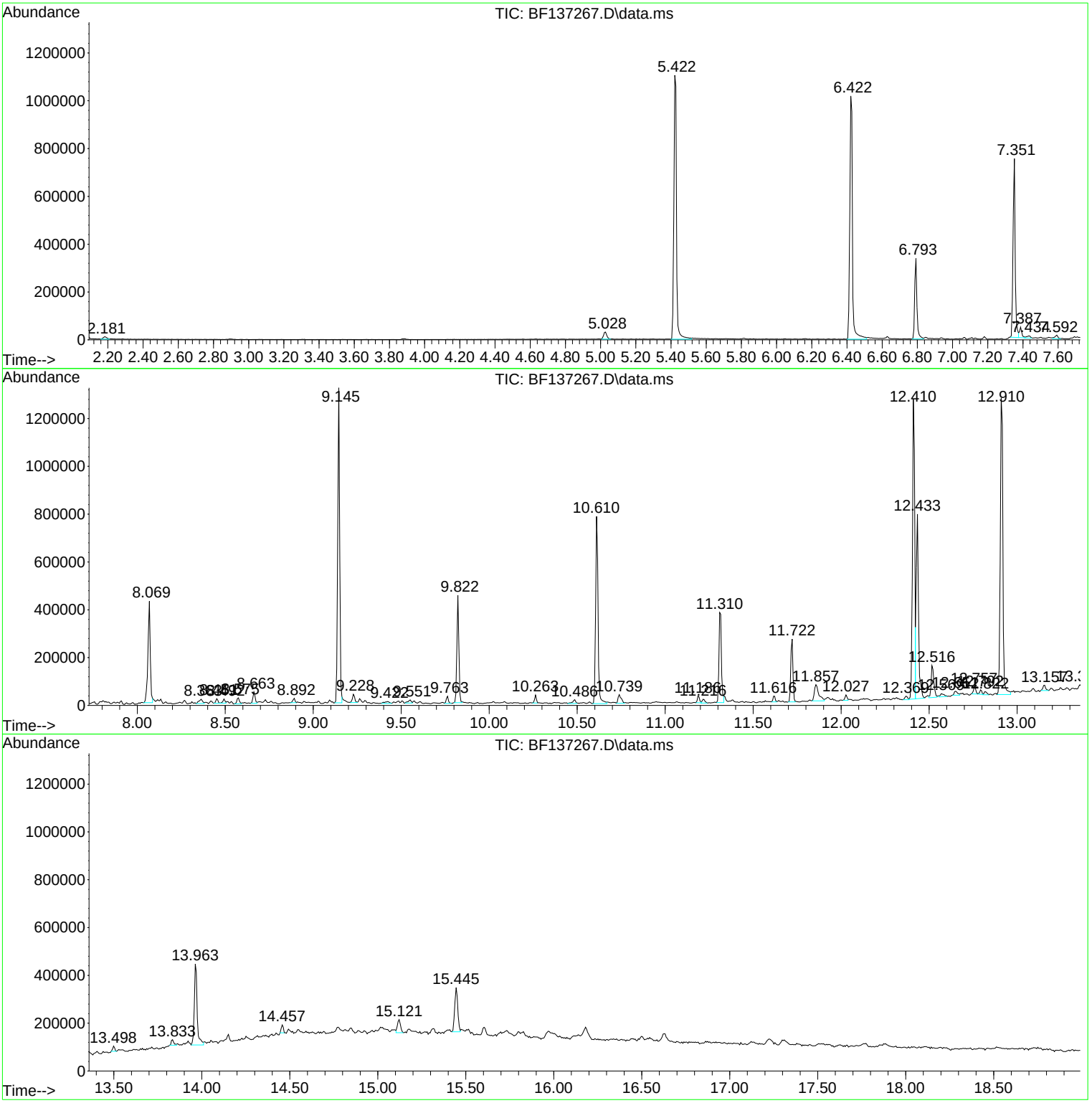
Sum of corrected areas: 10912076

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

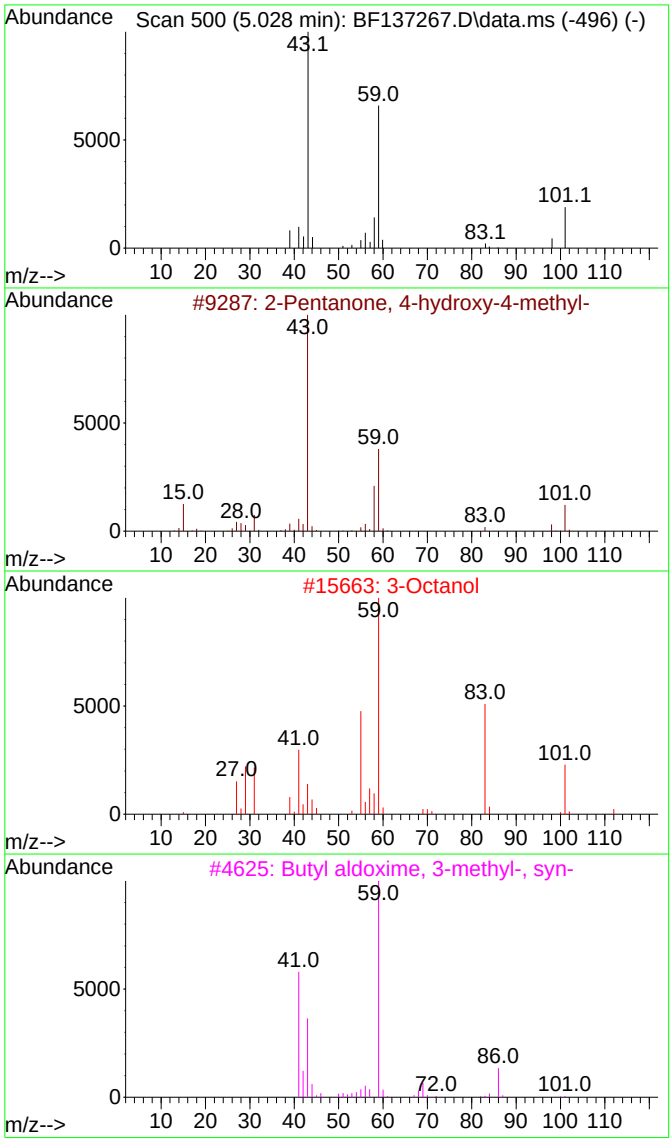
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

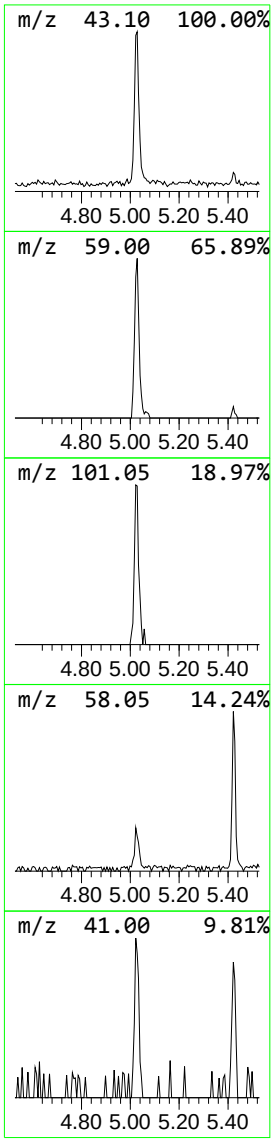
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	2.54 ng	37601	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

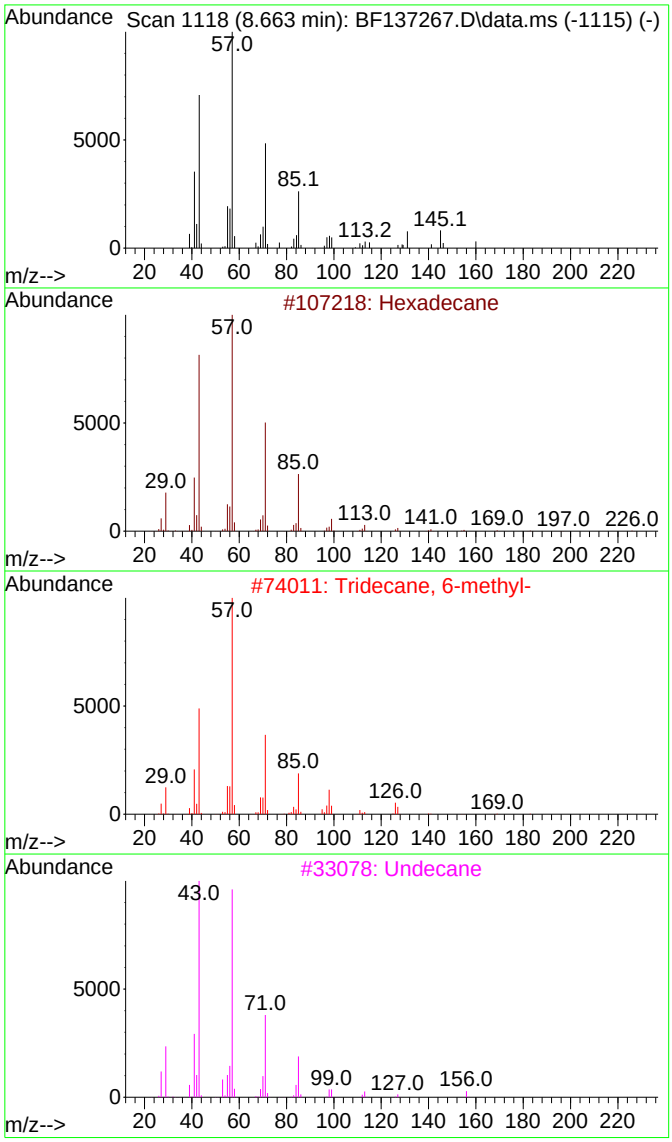
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

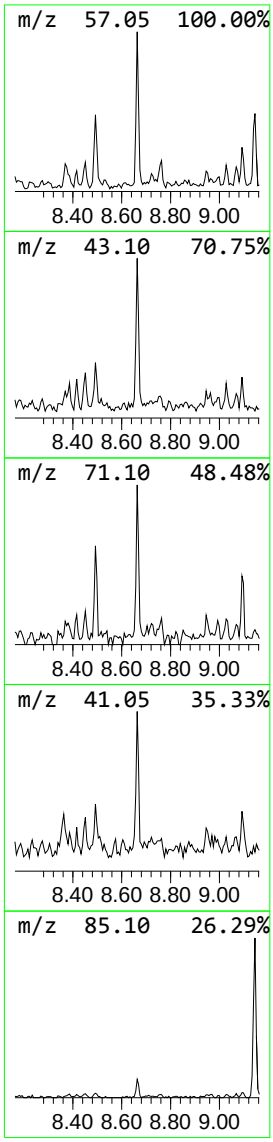
****

Peak Number 2 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	2.10 ng	40974	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
3	Undecane	156	C11H24	001120-21-4	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	Nonadecane	268	C19H40	000629-92-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

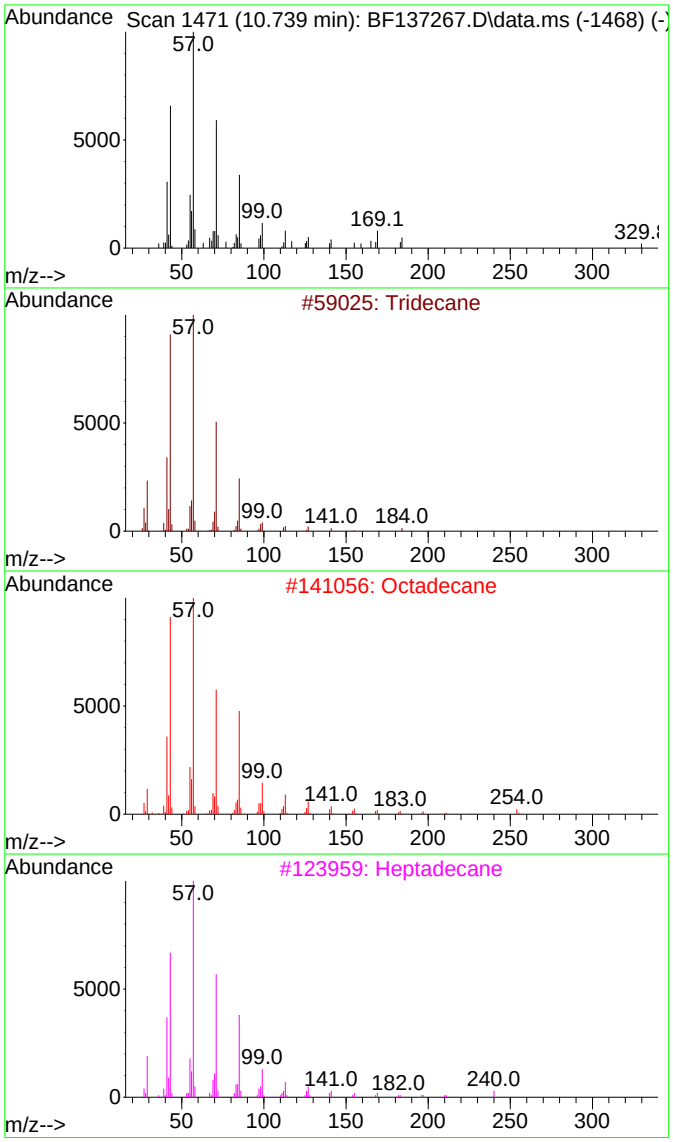
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

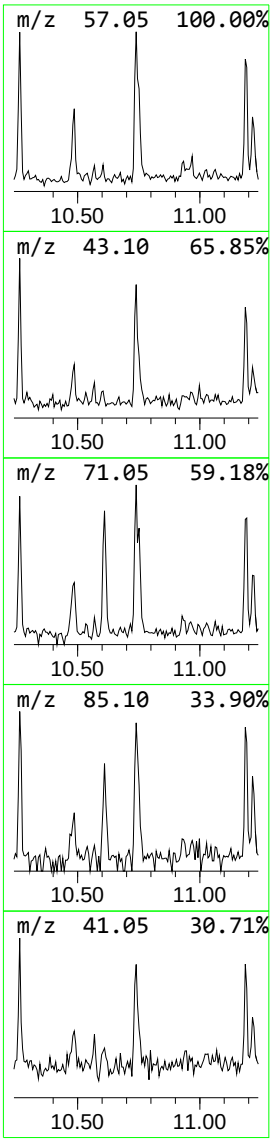
****

Peak Number 3 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	2.46 ng	45474	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Octadecane	254	C18H38	000593-45-3	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Heptacosane	380	C27H56	000593-49-7	83
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

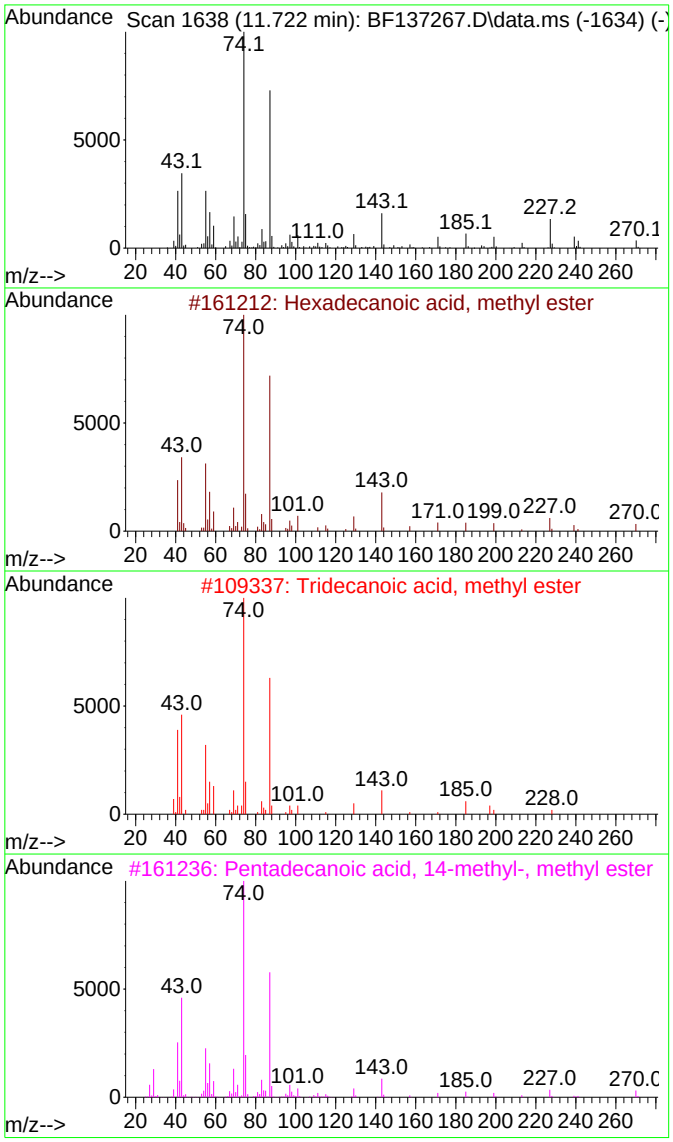
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

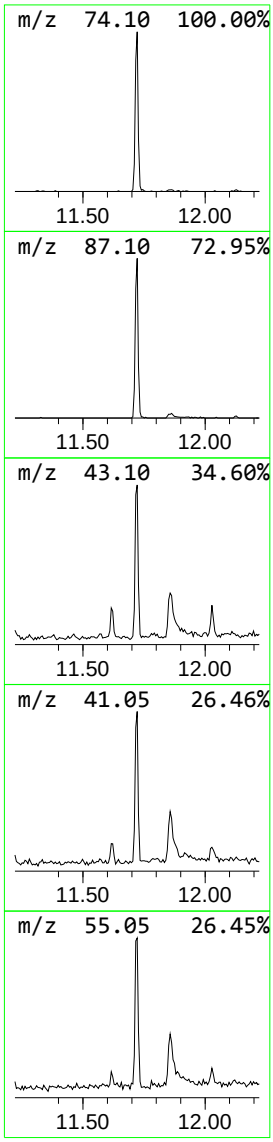
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.722	12.11 ng	223405	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

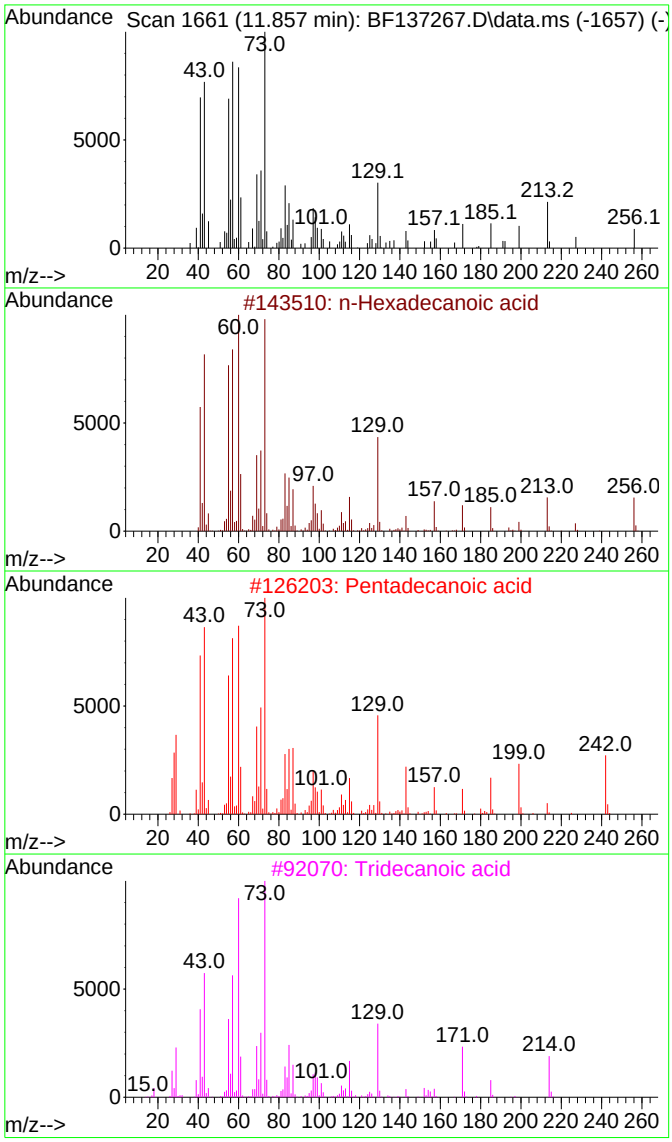
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

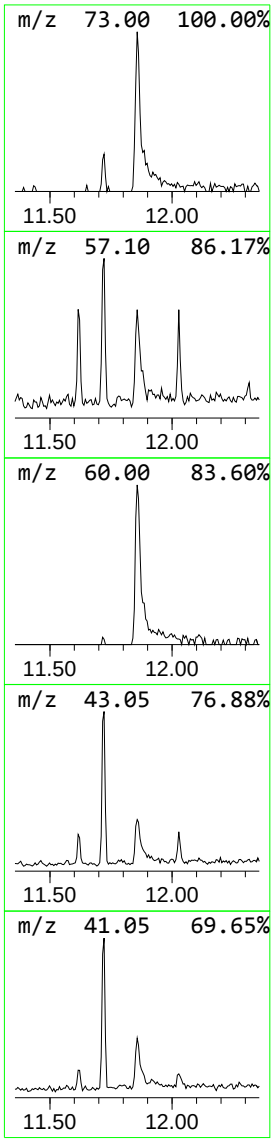
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	6.36 ng	117396	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Xylose	150	C5H10O5	000058-86-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

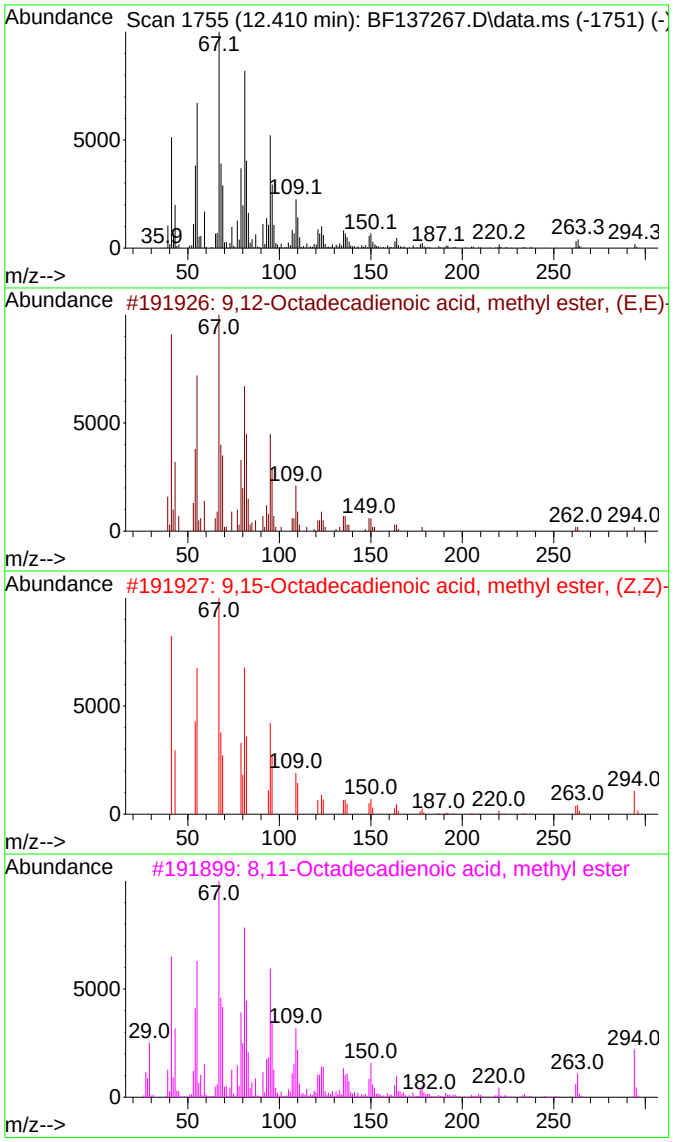
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

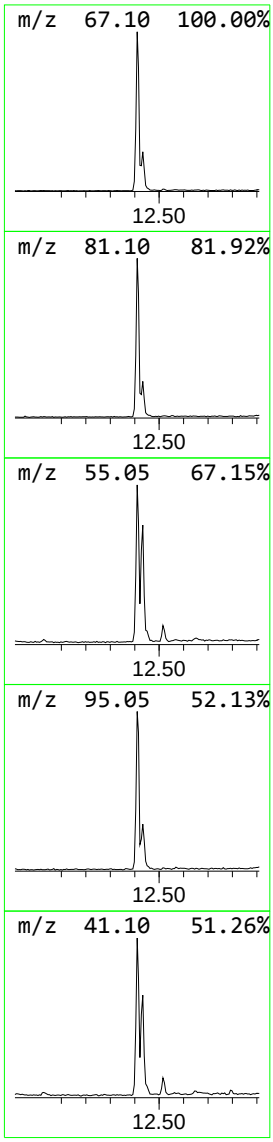
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	61.04 ng	1126240	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	97





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

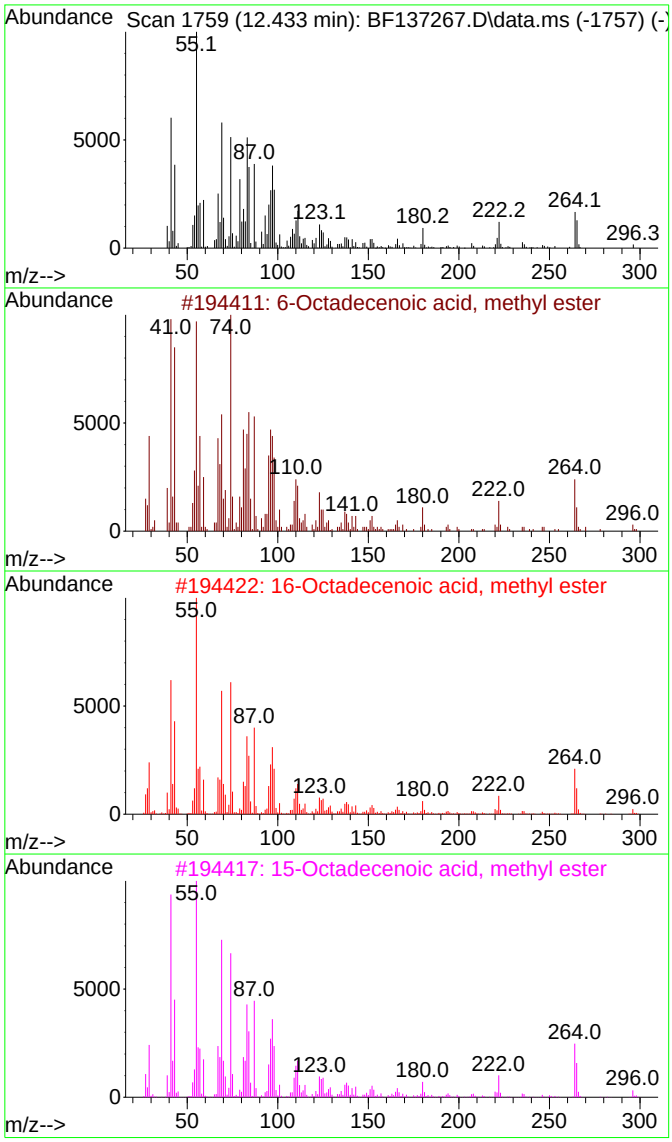
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

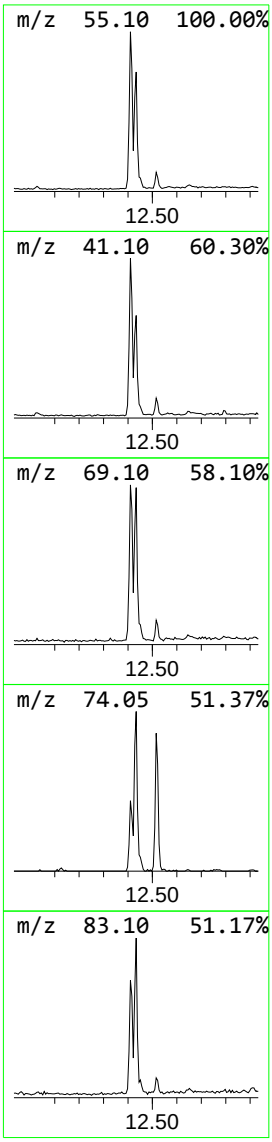
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 6-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	36.61 ng	675424	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

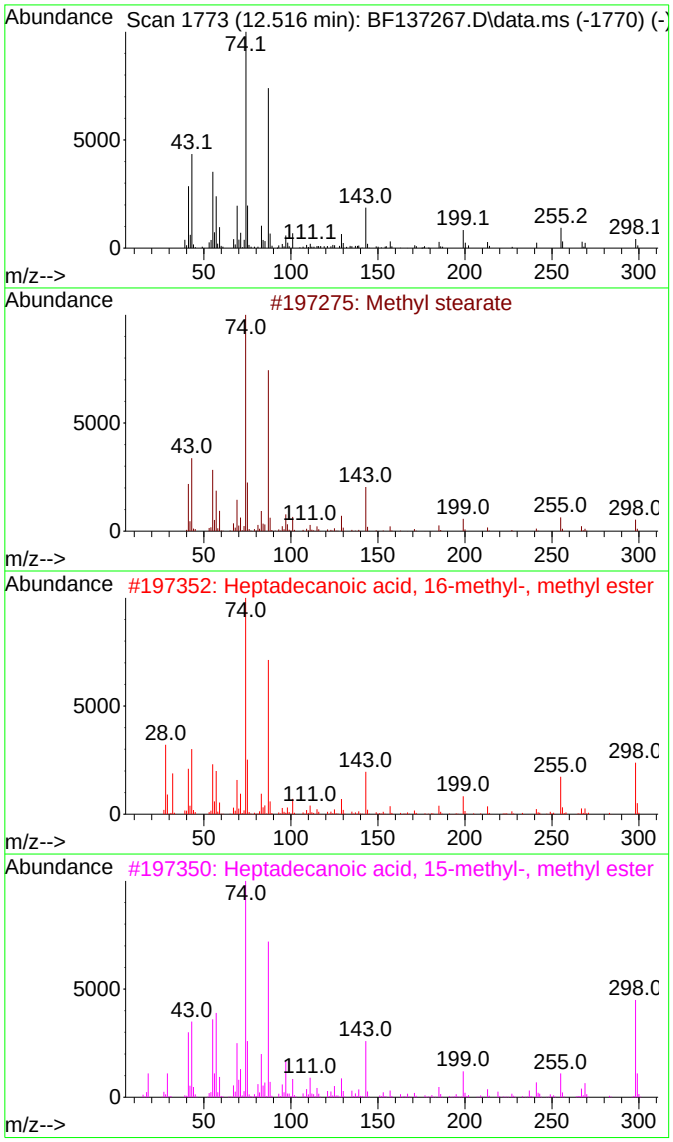
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

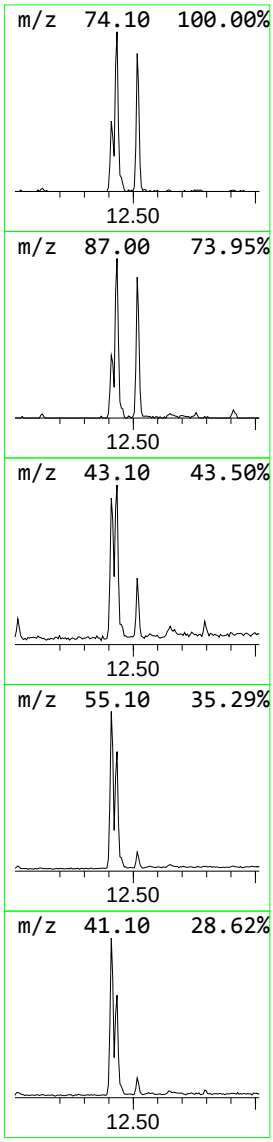
****

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.516	7.69 ng	141849	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

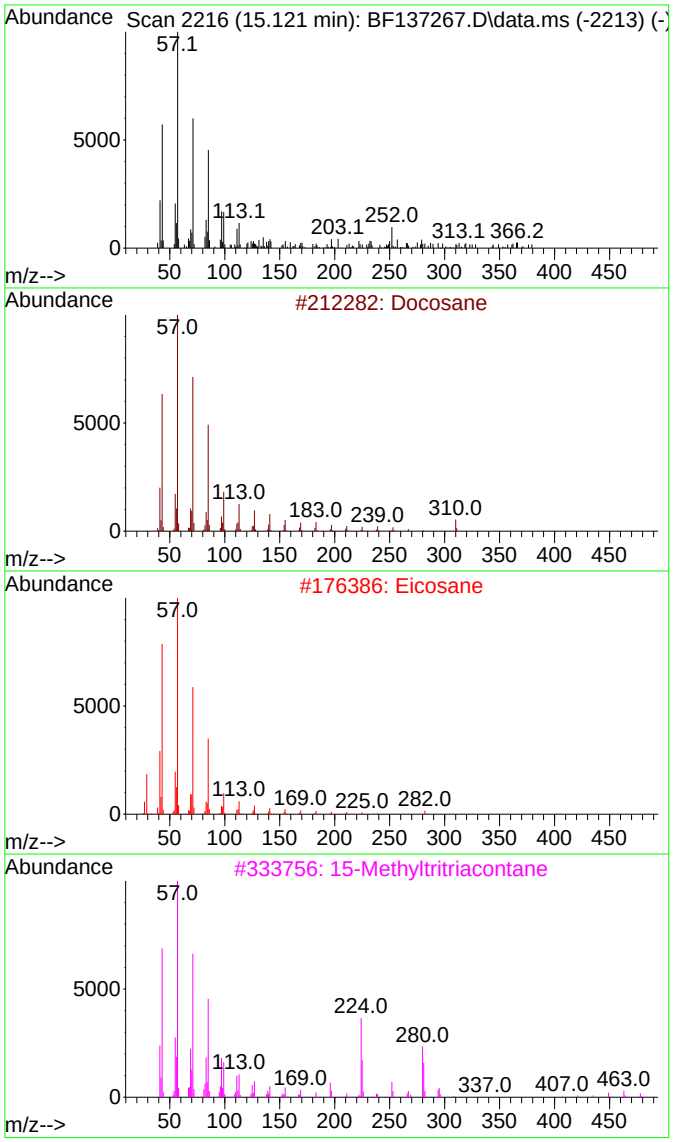
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

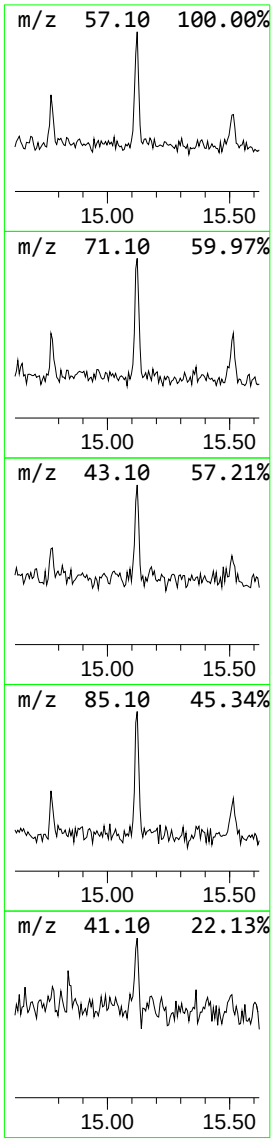
****

Peak Number 9 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	6.00 ng	64742	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	89
2	Eicosane	282	C20H42	000112-95-8	89
3	15-Methyltritriacontane	479	C34H70	1010131-20-3	72
4	Behenyl chloride	344	C22H45Cl	042217-03-8	68
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137267.D
Acq On : 02 Feb 2024 21:15
Operator : CG\JU
Sample : P1334-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-020124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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
2-Pentanone, 4-...	5.028	2.5	ng	37601	1	6.793	295841	20.0
Hexadecane	8.663	2.1	ng	40974	2	8.069	390061	20.0
Tridecane	10.739	2.5	ng	45474	4	11.316	369003	20.0
Hexadecanoic ac...	11.722	12.1	ng	223405	4	11.316	369003	20.0
n-Hexadecanoic ...	11.857	6.4	ng	117396	4	11.316	369003	20.0
9,12-Octadecadi...	12.410	61.0	ng	1126240	4	11.316	369003	20.0
6-Octadecenoic ...	12.433	36.6	ng	675424	4	11.316	369003	20.0
Methyl stearate	12.516	7.7	ng	141849	4	11.316	369003	20.0
Docosane	15.121	6.0	ng	64742	6	15.445	215836	20.0